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Electronic Supplementary Information

for

Reaction of Sulfur Ylides with Dienal and Enone: Insights on Chemo-, Regio-, and Diastereoselectivity Preferences

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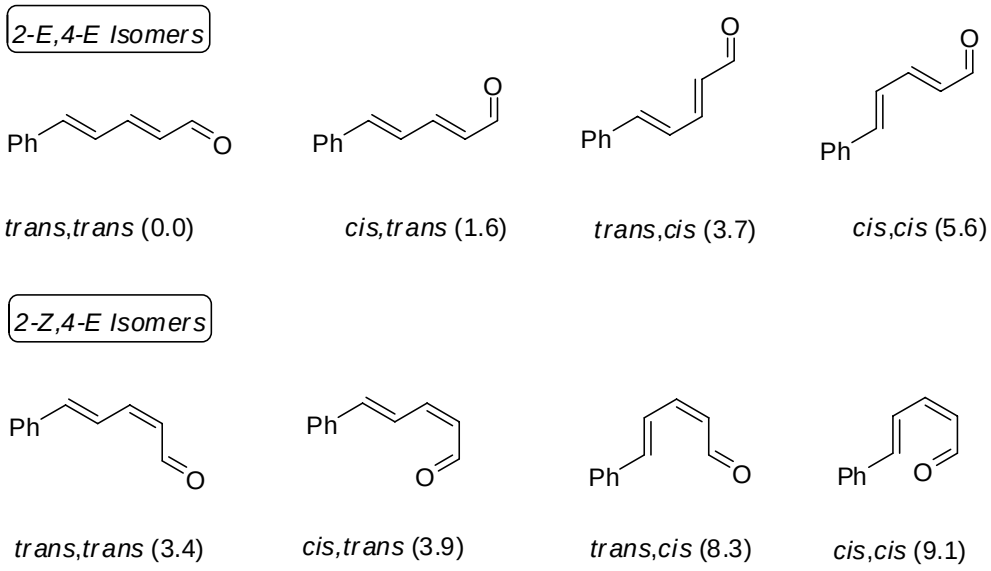
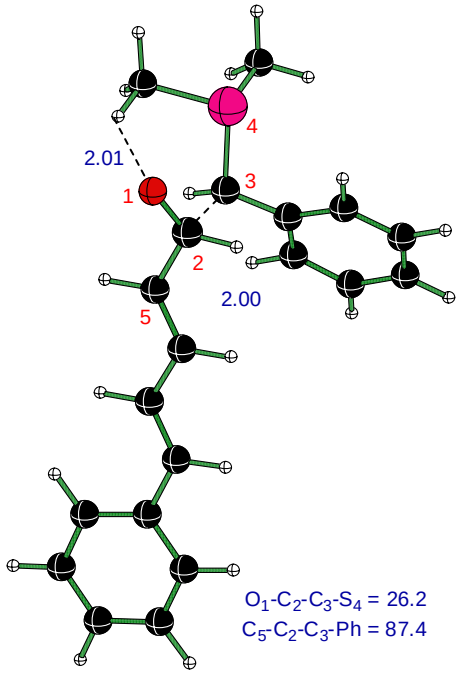


Fig. S1 Important Dienal Conformers and Their Relative Energies ΔE (in kcal mol^{-1}) obtained at the PCM$_{(MeCN)}$//B3LYP/6-311G**//B3LYP/6-31+G* Level of Theory. The notations *trans* and *cis* denote the s-*trans* and s-*cis* arrangement of adjacent double bonds but not the substituents around the C=C bonds.

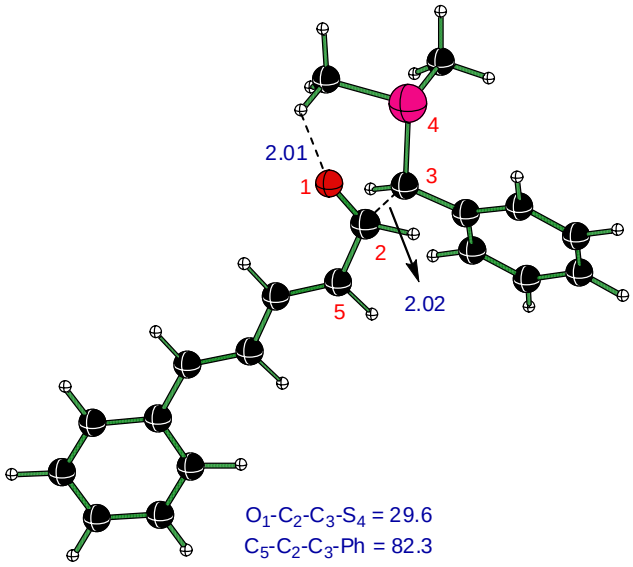
Table S1. Activation Barriers for the Elimination Steps Along Various Pathways in the Reaction between Dimethylsulfonium Benzylide and Dienal Computed at the PCM$_{(MeCN)}$//B3LYP/6-311G**//B3LYP/6-31+G* Level of Theory[a]

Pathway	**n**-E‡
1a	-1.3
1b	0.5
2a	3.1
2b	1.7
3a	5.5
3b	4.3

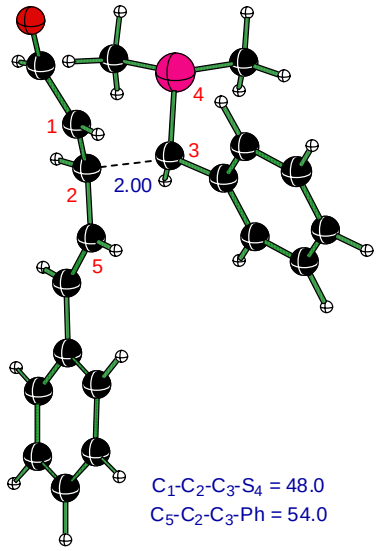
[a] $\Delta E^{‡}$ in kcal mol^{-1} relative to corresponding betaine intermediates.



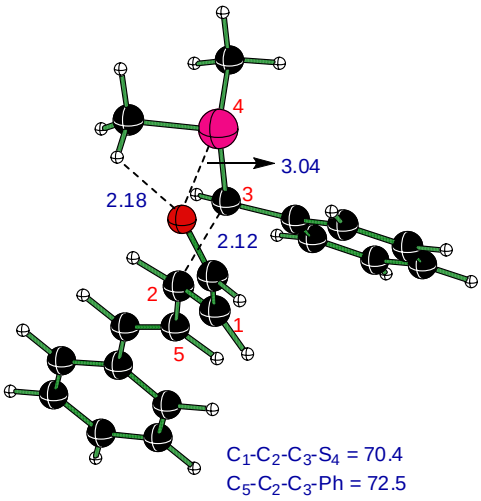
1a-A-$c^{‡}$ (*Out*) [*E*,*E*-*trans*,*trans*] (6.8)



1a-A-$c^{‡}$ (*Out*) [*E*,*E*-*cis*,*trans*] (4.0)



2b-A-$c^{‡}$ (*Out*) [*E*,*E* -*trans*,*trans*] (14.0)



2b-A-$c^{‡}$ (*Out*) [*E*,*E* -*cis*,*trans*] (9.9)

Fig. S2 The B3LYP/6-31+G* Optimized Geometries and Relative Energies ($\Delta E^{‡}$) of Selected Addition TSs (*In* and *Out* conformers) Computed with *E*,*E*-*cis*,*trans* Isomer of Dienal for the Reaction of Dimethylsulfonium Benzylide and Dienal (Distances in Å and angles in º). [$\Delta E^{‡}$ in kcal mol^{-1} obtained at the PCM$_{(MeCN)}$//B3LYP/6-311G**//B3LYP/6-31+G*; Energies relative to separated reactants]

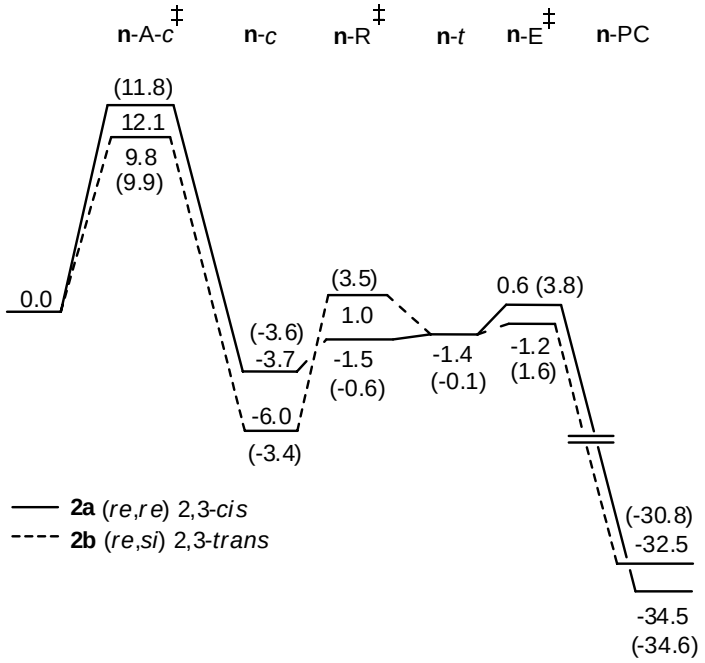
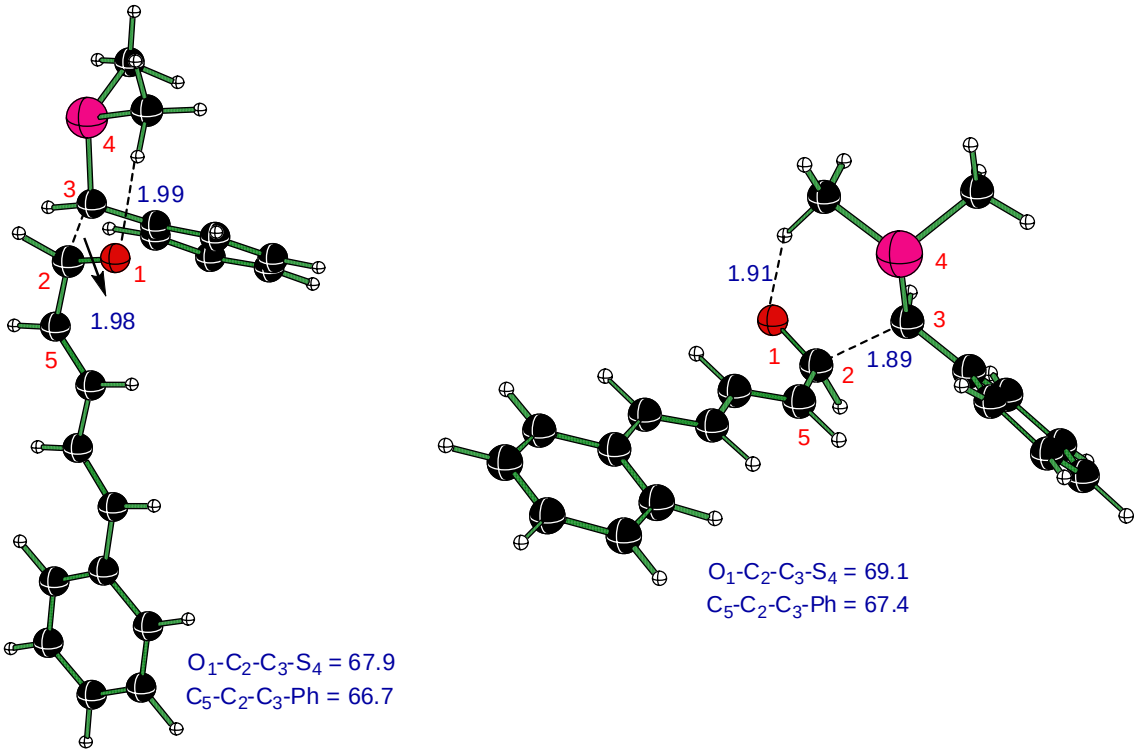


Fig. S3 The Reaction Energy Profiles for the 1,4-Addition Pathways for the Reaction Between Dimethylsulfonium Benzylide and Dienal Computed at the $PCM_{(MeCN)}$/B3LYP/6-311G**//HF/6-31+G* Level of Theory ($\Delta E^{\ddagger}$ in kcal mol^{-1} relative to reactants; corresponding energy values from the DFT method are provided in parentheses).



1b-A-*c*‡ (*In*) [*E*,*E*-*cis*,*trans* dienal] (5.5) **1b**-A-*c*‡ (*Out*) [*E*,*E*-*cis*,*trans* dienal] (4.2)

Fig. S4 The B3LYP/6-31+G* Optimized Geometries and Relative Energies ($\Delta E^{\ddagger}$) of Selected Addition TSs (*In* and *Out* conformers) Computed with *E*,*E*-*cis*,*trans* Isomer of Dienal for the Reaction of Dimethylsulfonium Benzylide and Dienal (Distances in Å and angles in º). [$\Delta E^{\ddagger}$ in kcal mol^{-1} obtained at the PCM$_{(MeCN)}$//B3LYP/6-311G**//B3LYP/6-31+G* level; Energies relative to separated reactants]

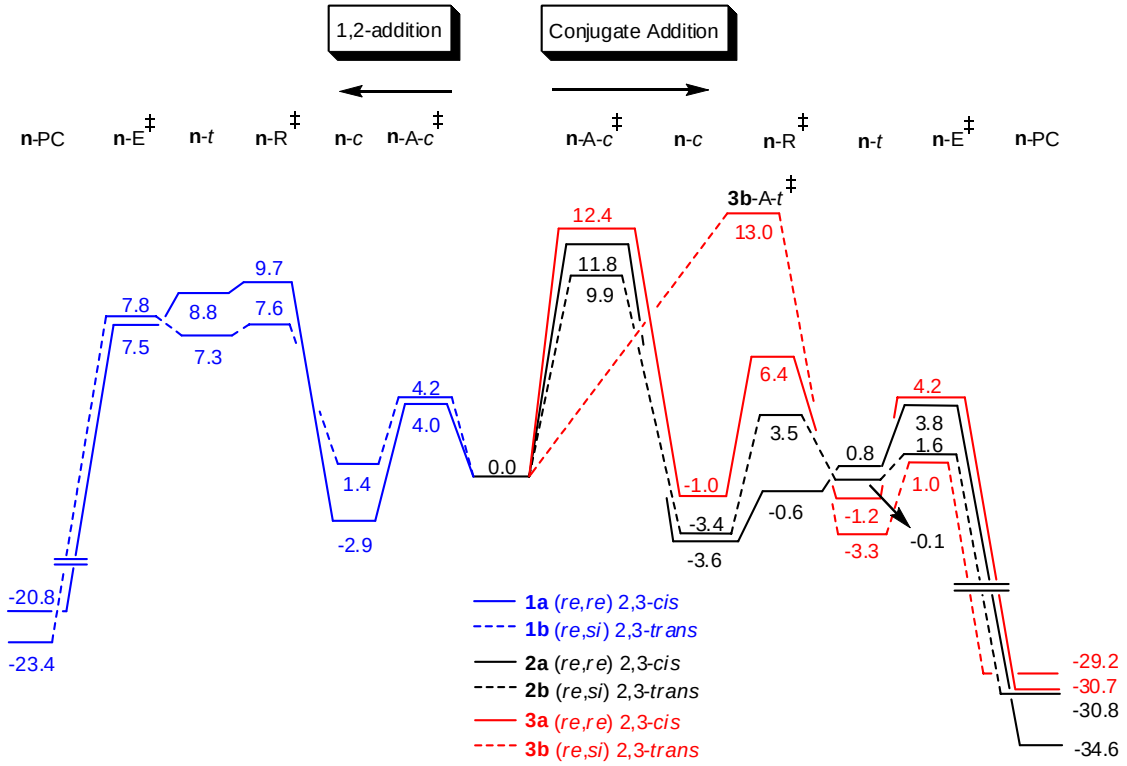
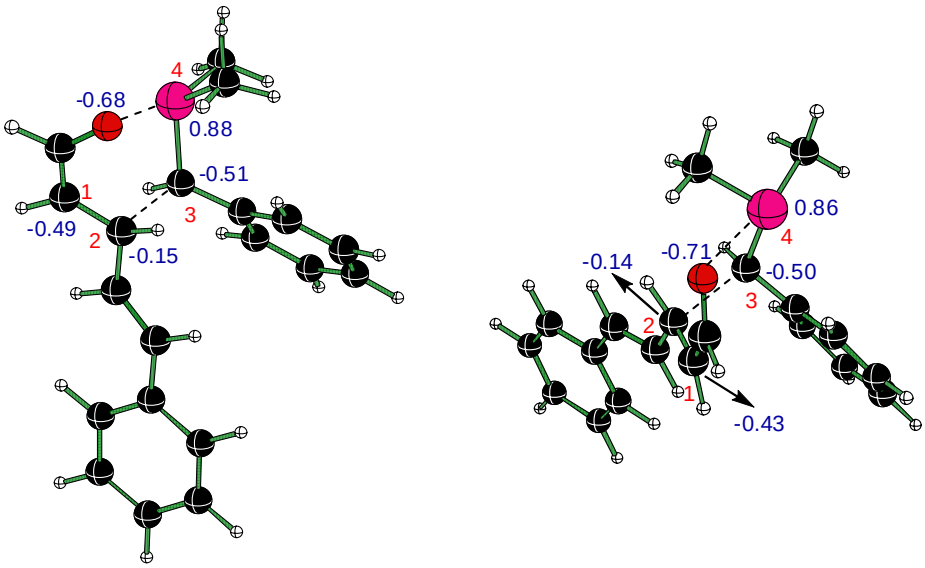


Fig. S5 Reaction Energy Profiles for All Diastereomeric Pathways for Direct and Conjugate Addition Modes for the Reaction Between Dimethylsulfonium Benzylide and Dienal Computed at the $PCM_{(MeCN)}$/B3LYP/6-311G**//B3LYP/6-31+G* Level ($\Delta E^{\ddagger}$ in kcal mol^{-1} relative to reactants).



2a-A-*c*‡ (11.8) **2b**-A-*c*‡ (9.9)

Fig. S6 The natural charges of selected atoms computed for diastereomeric addition TSs along the 1,4- pathway obtained at the B3LYP/6-311+G**//B3LYP/6-31+G* level of theory.

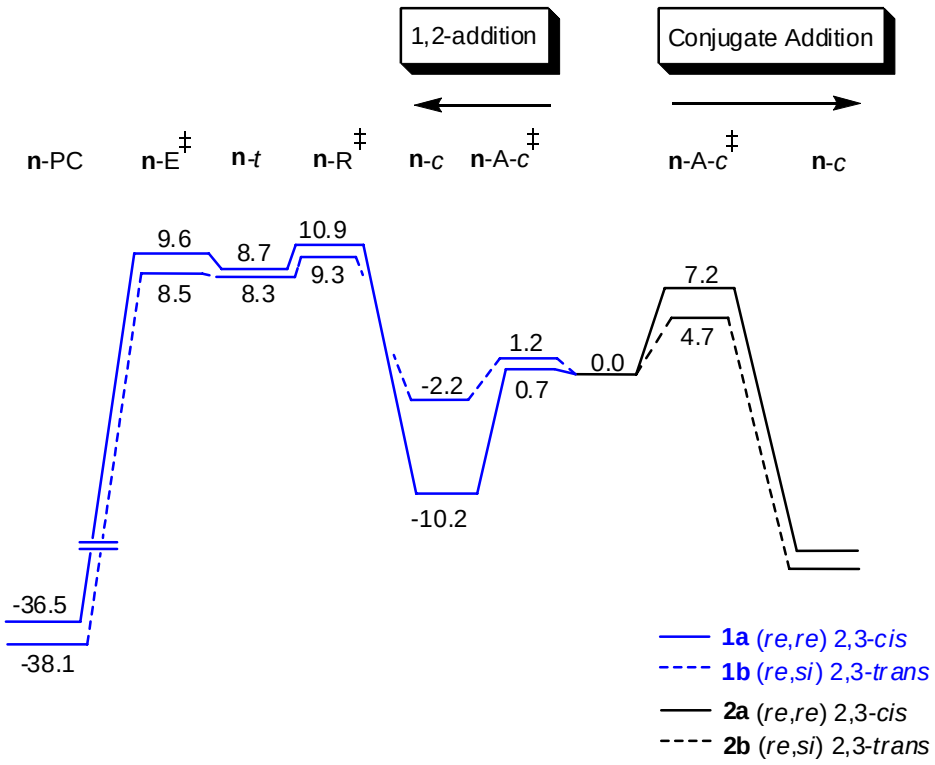


Fig. S7 Reaction Energy Profiles for Various Stationary Points on 1,2- and 1,4-Addition Pathways for the Reaction Between Dimethylsulfonium Benzylide and Dienal Computed at the mPW1K/6-311+G**//mPW1K/6-31+G* Level ($\Delta E^{\ddagger}$ in kcal mol^{-1} relative to reactants; Only the rate-limiting TSs are computed along the 1,4-pathway).

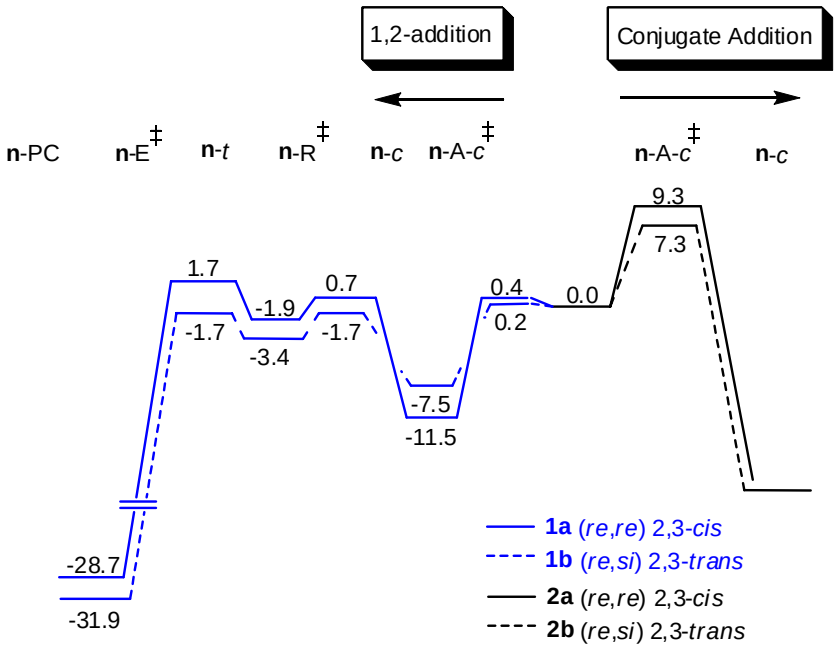


Fig. S8 Reaction Energy Profiles for Various Stationary Points on 1,2- and 1,4-Addition Pathways for the Reaction Between Dimethylsulfonium Benzylide and Dienal Computed at the $PCM_{(MeCN)}$/mPW1K/6-311G**//mPW1K/6-31+G* Level ($\Delta E^{\ddagger}$ in kcal mol^{-1} relative to reactants; only the rate-limiting TSs are computed for the 1,4-addition pathway).

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Table S2. The Natural Atomic Charges (in electron units) of Addition TSs Computed at the B3LYP/6-311+G**//B3LYP/6-31+G* Level for the addition of Dimethylsulfonium Benzylide to Dienal and Enone

TS	NPA charges				
	O_1	C_2	C_3	S_4	
1a-A-*c*‡	–0.79	0.27	–0.51	0.83	
1a-A-*t*‡	–0.78	0.20	–0.41	0.78	
1b-A-*c*‡	–0.81	0.23	–0.47	0.83	
1b-A-*t*‡	–0.78	0.21	–0.43	0.78	
	O	C_1	C_2	C_3	S_4
2a-A-*c*‡	–0.68	–0.49	–0.15	–0.51	0.88
2a-A-*t*‡	–0.71	–0.44	–0.14	–0.50	0.81
2b-A-*c*‡	–0.71	–0.43	–0.14	–0.50	0.86
2b-A-*t*‡	–0.65	–0.45	–0.16	–0.48	0.80
3a-A-*c*‡	–0.66	–0.35	–0.12	–0.50	0.84
3a-A-*t*‡	–0.64	–0.35	–0.15	–0.45	0.80
3b-A-*c*‡	–0.64	–0.37	–0.14	–0.46	0.82
3b-A-*t*‡	–0.63	–0.35	–0.16	–0.45	0.79
	O_1	C_2	C_3	S_4	
4a-A-*c*‡	–0.81	0.39	–0.49	0.82	
4a-A-*t*‡	–0.78	0.34	–0.42	0.77	
4b-A-*c*‡	–0.83	0.36	–0.45	0.82	
4b-A-*t*‡	–0.79	0.33	–0.41	0.75	
	O	C_1	C_2	C_3	S_4
5a-A-*c*‡	–0.71	–0.46	–0.07	–0.56	0.85
5a-A-*t*‡	–0.70	–0.47	0.19	–0.51	0.83
5b-A-*c*‡	–0.70	–0.49	–0.09	–0.55	0.86
5b-A-*t*‡	–0.72	–0.45	–0.09	–0.52	0.81

Table S3. Relative Energies of Addition TSs along the Conjugate Addition Pathway (**5**) for the Reaction Between Dimethylsulfonium Benzylide and Enone ($\Delta\Delta E^{\ddagger}$ in kcal mol^{-1})

Method	**5a**-A-*c*‡	**5a**-A-*t*‡	**5b**-A-*c*‡	**5b**-A-*t*‡
I	0.3	3.0	3.0	0.0
II	0.3	3.0	3.1	0.0

I: $PCM_{(MeCN)}$/B3LYP/6-311G**//B3LYP/6-31+G* level

II: $PCM_{(MeCN)}$/B3LYP/6-311G**//B3LYP/6-31+G** level

Table S4. Relative free energies incorporating Benson's corrections[a,b] to stationary points from pathway-**2** (Figure S10)

Pathway	**n**-A-*c*‡			**n**-E‡		
	$\Delta G_{sol}^{\ddagger}$	$\Delta G^{\ddagger 1atm}$	$\Delta G^{\ddagger 1M+FV}$	$\Delta G_{sol}^{\ddagger}$	$\Delta G^{\ddagger 1atm}$	$\Delta G^{\ddagger 1M+FV}$
1a	4.0	20.0	15.2	-	-	-
1b	4.2	21.6	16.8	-	-	-
2a	11.8	25.5	20.7	1.6	25.4	20.6
2b	9.9	23.9	19.1	3.8	-	-

[a] $\Delta G_{sol}^{\ddagger} = [E_X + G_{corr(X)}] - [E_R + G_{corr(R)}]$ (Unscaled)

Where E_X and E_R denote the free energies of solvation, and $G_{corr(X)}$ and $G_{corr(R)}$ denote the correction to free energy (from the gas phase calculations) for the stationary point X and the separated reactants R respectively.

[b] For bimolecular reactions, $\Delta G^{\ddagger 1M}$ lowers the free energies of the system by 1.89 kcal mol^{-1} and the $\Delta G^{\ddagger FV}$ correction (Benson's correction at 298 K for the standard state of 1M) causes a reduction of 2.96 kcal mol^{-1} from the corresponding gas phase corrected values (For details on the calculation of benson's corrections, see: (a) Alvarez-Idaboy, J. R.; Reyes, L.; Cruz, J. *Org. Lett.***2006**, *8*, 1763; (b) Galano, A. *J. Phys. Chem. A.* **2007**, *111*, 1677.)

Table S5. The Relative Energies of (in kcal mol^{-1}) TSs, Intermediates, and Products for the 1,2– (pathway-**1**), and addition TSs along 1,4– (pathway-**2**) computed using the mPW1K functional[a]

	n-A-*c*‡	**n**-A-*t*‡	**n**-*c*	**n**-*t*	**n**-R‡	**n**-E‡	**n**-PC
At the mPW1K/6-311+G**// mPW1K/6-31+G* level							
1a	0.7	9.8	-10.2	8.7	10.9	9.6	-36.5
1b	1.2	-[b]	-2.2	8.3	9.3	8.5	-38.1
2a[c]	7.2	-	-	-	-	-	-
2b[c]	4.7	-	-	-	-	-	-
At the PCM_{MeCN}/mPW1K/6-311G**/ mPW1K/6-31+G* level							
1a	0.4	3.2	-11.5	-1.9	0.7	1.7	-28.7
1b	0.2	-	-7.5	-3.4	-1.7	-1.7	-31.9
2a[c]	9.3	-	-	-	-	-	-
2b[c]	7.3	-	-	-	-	-	-

[a] $\Delta E^{\ddagger}$ relative to separated reactants; energies in kcal mol^{-1}

[b] Geometric convergence is not achieved

[c] For the 1,4- pathway, only the rate-limiting TSs are computed at the mPW1K/6-31+G* level.

Enthalpies and Free energies:

The relative enthalpies and free energies obtained at the B3LYP/6-31+G* level show different energy trends for the 1,4-addition pathway. Surprisingly, these values are highest for the torsional motion step, as opposed to the order revealed by the relative energies (and relative solvation free energies).

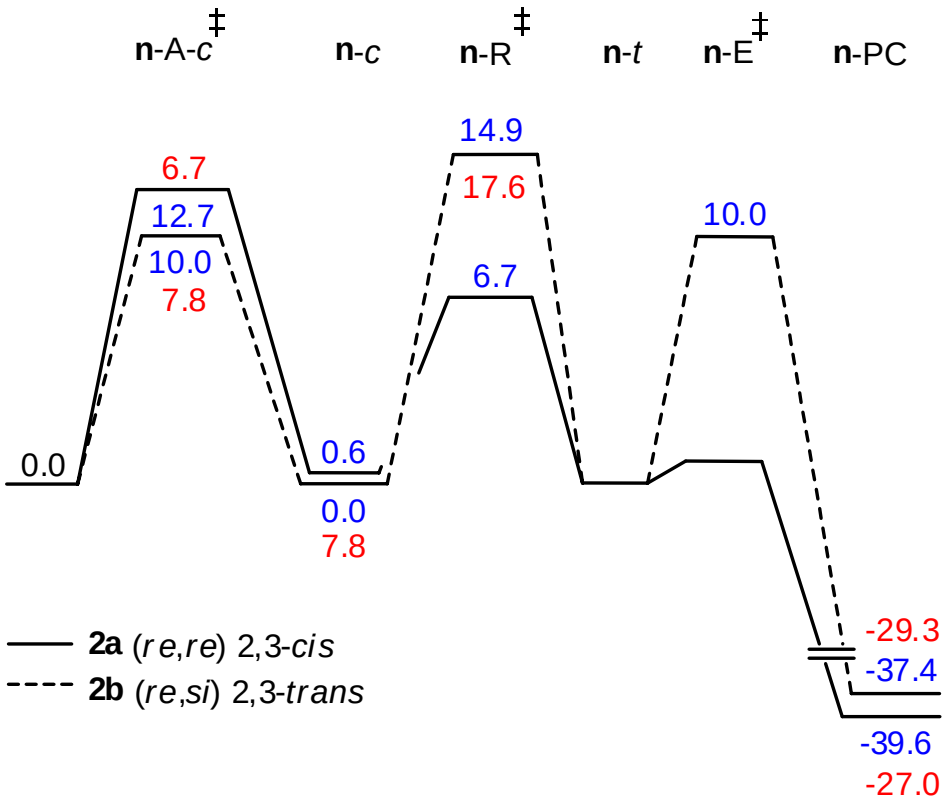

Fig. S9 Relative enthalpies of various stationary points along the diastereomeric 1,4-addition pathways (blue font) for the reaction between dimethylsulfonium benzylide and dienal obtained at the B3LYP/6-31+G* level (values in the red font are relative enthalpies along the 1,2-addition pathway)[stationary points **2a**-*t* and **2a**-E‡ have been optimized at the $PCM_{(MeCN)}$/B3LYP/6-31+G*and HF/6-31+G* levels respectively and hence the corrections cannot be included]

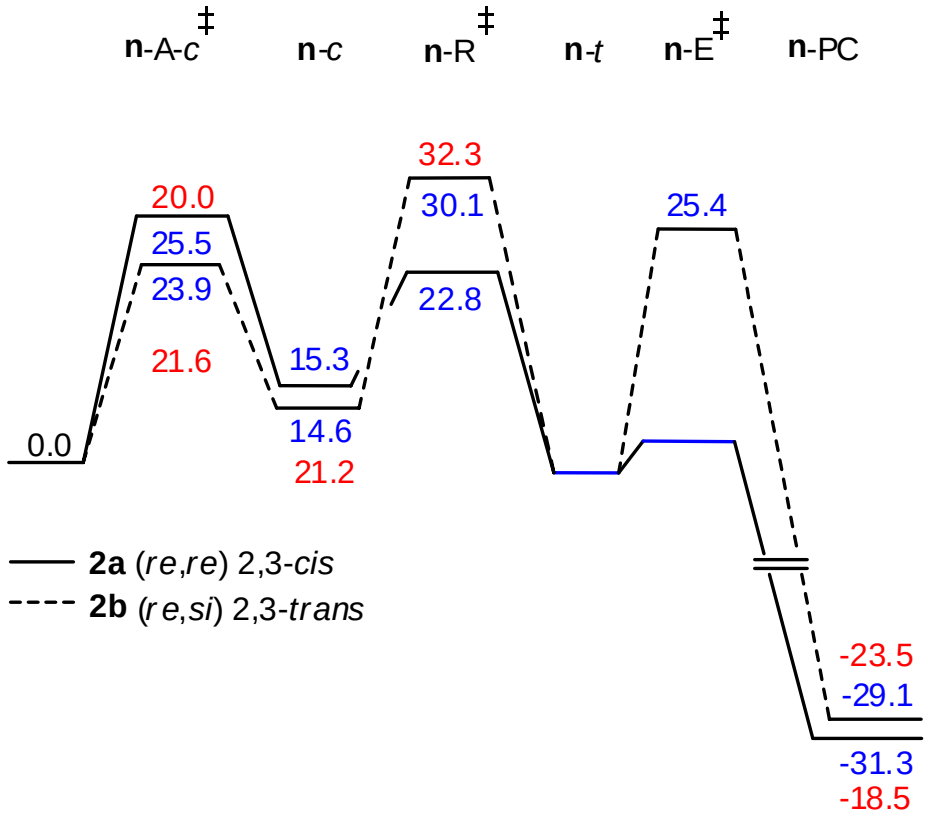

Fig. S10 Relative free energies of various stationary points (in blue font) along the diastereomeric 1,4-addition pathways for the reaction between dimethylsulfonium benzylide and dienal obtained at the B3LYP/6-31+G* level of theory (values in the red font are relative free energies along the 1,2-addition pathway). [stationary points **2a**-*t* and **2a**-E‡ have been optimized at the $PCM_{(MeCN)}$/B3LYP/6-31+G*and HF/6-31+G* levels respectively and hence the corrections cannot be included]

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Table S6. Relative energies (in kcal mol^{-1}). of selected stationary points from 1,4-addition pathway computed in acetonitrile at the B3LYP/6-31+G* level of theory

	ΔE (B1)	ΔE (B2)	ΔE (B2 + ZPE)	ΔE (B2 + Gcorr.)
Reactants	0.0	0.0	0.0	0.0
2a-A-*c*‡	11.8	11.1	12.3	24.6
2b-A-*c*‡	9.9	8.3	9.4	22.5
2b-*c*	-3.4	-6.3	-3.0	10.9
2b-*t*	-0.1	-1.6	1.4	14.9

B1: $PCM_{(MeCN)}$/B3LYP/6-311G**//B3LYP/6-31+G* level ; B2: $PCM_{(MeCN)}$/B3LYP/6-311G**//$PCM_{(MeCN)}$/B3LYP/6-31+G* level; Energies are relative to the separated reactants.

Optimized Cartesian coordinates and energies of TSs, intermediates, reactants and products obtained at the B3LYP/6-31+G* level (Energy in a. u.). Single-point energies (at the PCM $_{(MeCN)}$/B3LYP/6-311G**//B3LYP/6-31+G* level), imaginary frequencies, if any (in cm^{-1}), are also given after the respective coordinates. In cases where B3LYP/6-31+G* geometries could not be obtained, geometries obtained at either PCM $_{(MeCN)}$/B3LYP/6-31+G* level or HF/6-31+G* level are provided.

I. Addition to Dienal

1,2-addition (Pathway 1)

1. **1a**-A-$c^{‡}$ conformer 1 (-1248.701119)

6	2.595568	-3.162756	0.842753
16	3.587448	-1.758387	0.252130
6	2.392309	-0.412320	0.263930
6	4.679738	-1.490105	1.701929
6	1.298833	-0.918229	-1.355166
6	0.042953	-0.190255	-0.987660
1	2.206736	-2.942162	1.840835
1	1.795907	-3.260687	0.099897
1	4.081720	-1.390978	2.611309
1	5.242709	-0.571998	1.521283
1	1.757078	-0.529009	1.145381
1	5.366515	-2.338644	1.779632
1	3.240362	-4.044793	0.857609
6	3.006482	0.923935	0.139857
6	3.975669	1.224213	-0.843341
6	4.478374	2.518336	-0.987229
6	4.017377	3.555268	-0.170256
6	3.046288	3.278955	0.797966
6	2.555249	1.982908	0.956745
1	4.329483	0.441259	-1.510806
1	5.225592	2.718836	-1.751413
1	4.405639	4.563245	-0.288795
1	2.675420	4.074378	1.440134
1	1.806063	1.781260	1.719592
1	0.119911	0.892635	-0.874408
6	-1.147558	-0.809617	-0.836925
6	-2.385148	-0.133468	-0.511350
1	-1.177168	-1.889162	-0.985640
1	-2.324664	0.947763	-0.382315
6	-3.575156	-0.765175	-0.367435
1	-3.589037	-1.847626	-0.502573
6	-4.872970	-0.166860	-0.044422
6	-5.992018	-1.010140	0.110553
6	-7.252672	-0.498026	0.419870
6	-7.430338	0.878374	0.581834
6	-6.331382	1.732940	0.428970
6	-5.073379	1.220402	0.120562
1	-5.863998	-2.083474	-0.014524
1	-8.096275	-1.174704	0.533118
1	-8.410523	1.282507	0.821345
1	-6.457966	2.806431	0.548508
1	-4.238956	1.905856	0.001884
1	1.940700	-0.304321	-2.023032
8	1.299533	-2.181586	-1.523526

$E_{(MeCN)}$ = -1248.923357
NImag = 1 (-226.4)

2. **1a**-A-$c^{‡}$ conformer 2 (-1248.699164)

6	5.419927	0.103040	1.221359
6	5.060802	-0.247997	-0.097426
6	6.083206	-0.272192	-1.067593
6	7.403604	0.040171	-0.741751
6	7.739179	0.386700	0.569495
6	6.737608	0.415139	1.547982
6	3.693171	-0.582585	-0.503191
6	2.582730	-0.615032	0.272130
6	1.265759	-0.955350	-0.224035
6	0.151082	-1.011089	0.535908
6	-1.194065	-1.400672	-0.014768
6	-2.291440	0.143500	0.605325
6	-3.744837	-0.168274	0.511409
6	-4.300339	-0.757003	-0.643201
6	-5.658687	-1.079948	-0.692723
6	-6.489156	-0.838501	0.405910
6	-5.946562	-0.279694	1.567170
6	-4.591604	0.053778	1.615905
16	-1.700216	1.582402	-0.288545
6	-1.849591	1.168149	-2.058562
6	-2.952253	2.922478	-0.176804
8	-1.332420	-1.619094	-1.261536

1	-3.941200	2.527340	-0.420424
1	-2.939316	3.307910	0.845180
1	-2.901876	1.153090	-2.351261
1	-1.409041	0.166994	-2.166214
1	-1.967354	0.330818	1.633028
1	-1.297899	1.929920	-2.614701
1	-2.664595	3.713222	-0.876449
1	-3.642961	-1.020975	-1.465583
1	-6.065005	-1.543285	-1.588710
1	-7.544407	-1.096207	0.363429
1	-6.577613	-0.101490	2.434693
1	-4.178433	0.488883	2.524318
1	0.209640	-0.815531	1.609172
1	1.165373	-1.198678	-1.281938
1	2.653323	-0.377162	1.334088
1	3.575739	-0.832860	-1.558531
1	5.831759	-0.542115	-2.091296
1	8.170052	0.011855	-1.512488
1	8.766193	0.630626	0.828629
1	6.987198	0.681737	2.572316
1	4.662356	0.131539	1.999475
1	-1.740314	-2.059017	0.697035

$E_{(MeCN)}$ = -1248.923071
NImag = 1 (-217.9)

3. **1a**-A-*c*‡ conformer 3 (-1248.699859)

6	4.142744	-2.673692	0.735782
16	4.207312	-0.959232	0.134016
6	2.493884	-0.424531	0.311272
6	5.133702	-0.161642	1.501973
6	1.655093	-1.413631	-1.208010
6	0.270696	-1.566880	-0.663858
1	3.795945	-2.685433	1.773024
1	3.440501	-3.170288	0.056355
1	4.654945	-0.379199	2.459997
1	5.128083	0.914428	1.316269
1	2.105148	-0.837768	1.245988
1	6.161821	-0.536487	1.488587
1	5.147416	-3.095428	0.653163
6	2.316885	1.035302	0.191457
6	2.922214	1.791175	-0.837457
6	2.665218	3.156053	-0.974669
6	1.780612	3.803345	-0.106019
6	1.157109	3.065601	0.905349
6	1.427094	1.705168	1.057352
1	3.589887	1.304539	-1.545661
1	3.149233	3.713079	-1.773448
1	1.576870	4.864828	-0.218803
1	0.461398	3.551979	1.585018
1	0.936789	1.145086	1.850240
1	0.106650	-2.471116	-0.074580
6	-0.748664	-0.712497	-0.900926
6	-2.096643	-0.886865	-0.400238
1	-0.562420	0.170999	-1.514292
1	-2.273315	-1.781839	0.196766
6	-3.108432	-0.017122	-0.633090
1	-2.885255	0.865718	-1.234048
6	-4.494473	-0.110773	-0.167088
6	-5.394623	0.922737	-0.496633
6	-6.725600	0.889499	-0.078782
6	-7.195084	-0.183818	0.682570
6	-6.316489	-1.221500	1.018248
6	-4.987964	-1.186821	0.601056
1	-5.038429	1.762498	-1.089941
1	-7.395837	1.701932	-0.349103
1	-8.231172	-0.214906	1.009653
1	-6.671231	-2.063551	1.607906
1	-4.327977	-2.006079	0.871941
1	1.736875	-0.548468	-1.899114
8	2.336676	-2.463932	-1.473739

$E_{(MeCN)}$ = -1248.921522
NImag = 1 (-249.0)

4. **1a**-A-*c*‡ conformer 4 (-1248.697435)

6	-5.526488	-0.811104	0.034433
6	-4.981576	0.487815	-0.049879
6	-5.845830	1.575208	0.189740
6	-7.191649	1.380290	0.502661
6	-7.712344	0.086320	0.583357
6	-6.869927	-1.007018	0.346182
6	-3.577513	0.758196	-0.370394
6	-2.592501	-0.141397	-0.604121
6	-1.223608	0.221511	-0.910124
6	-0.224477	-0.659099	-1.131308
6	1.181055	-0.274609	-1.503811
6	2.044395	-0.120951	0.256050
6	3.272509	0.722089	0.192890
6	4.205615	0.580033	-0.854830
6	5.324736	1.412987	-0.927657
6	5.533407	2.410375	0.030006
6	4.603361	2.579376	1.060273
6	3.488215	1.742647	1.140286
16	2.244726	-1.798036	0.870709
6	3.320036	-2.637479	-0.338552
6	3.360698	-1.788539	2.330870

8	1.827560	-1.049836	-2.290377
1	4.259868	-1.209401	2.107402
1	2.816444	-1.337691	3.163821
1	4.327935	-2.218452	-0.297598
1	2.855232	-2.443692	-1.315452
1	1.271415	0.298950	0.904898
1	3.324484	-3.699918	-0.083096
1	3.614526	-2.825734	2.570648
1	4.006815	-0.144560	-1.639261
1	6.026752	1.293956	-1.749568
1	6.403889	3.058439	-0.033618
1	4.745270	3.361992	1.801853
1	2.767447	1.884485	1.943698
1	-0.424297	-1.732105	-1.113936
1	-1.003397	1.290218	-0.970652
1	-2.807924	-1.209324	-0.566302
1	-3.314847	1.816180	-0.419189
1	-5.449761	2.586868	0.128241
1	-7.833206	2.239581	0.682402
1	-8.760123	-0.071084	0.825771
1	-7.264763	-2.018665	0.403063
1	-4.895524	-1.676330	-0.148709
1	1.268986	0.823658	-1.659169

$E_{(MeCN)}$ = -1248.920358
NImag = 1 (-228.2)

5. **1a**-A-$t^{‡}$ conformer 1 (-1248.686046)

6	3.701702	-3.091399	-0.113624
16	3.275130	-1.517921	-0.927520
6	2.915887	-0.406092	0.513301
6	4.924545	-1.061354	-1.597216
6	1.734774	-0.958100	1.697145
6	0.427863	-1.185806	0.964689
1	4.438963	-2.922995	0.675531
1	2.788054	-3.503293	0.316849
1	5.662712	-1.050245	-0.790984
1	4.822962	-0.063454	-2.028464
1	3.831469	-0.414307	1.113194
1	5.206072	-1.778753	-2.373801
1	4.094518	-3.769005	-0.875879
6	2.618540	0.968543	-0.006154
6	1.727563	1.207322	-1.067970
6	1.428663	2.510480	-1.470010
6	1.997319	3.600911	-0.805004
6	2.865311	3.376256	0.266497
6	3.178322	2.072679	0.657670
1	1.244227	0.374883	-1.572771
1	0.736743	2.672528	-2.292750
1	1.757073	4.615319	-1.113159
1	3.298064	4.216201	0.804157
1	3.834655	1.902753	1.505979
1	0.395186	-2.004620	0.235509
6	-0.684465	-0.466887	1.213286
6	-1.963665	-0.680322	0.568008
1	-0.604386	0.322762	1.960107
1	-2.011444	-1.496057	-0.155081
6	-3.066876	0.065300	0.815428
1	-2.973568	0.873261	1.542098
6	-4.395969	-0.075469	0.214044
6	-5.406542	0.839177	0.573788
6	-6.690012	0.756940	0.032165
6	-7.001003	-0.248391	-0.887055
6	-6.011543	-1.168714	-1.254824
6	-4.730547	-1.084924	-0.713826
1	-5.174358	1.625185	1.289450
1	-7.447408	1.478314	0.329541
1	-7.999721	-0.317499	-1.310527
1	-6.242335	-1.958054	-1.966579
1	-3.982860	-1.814618	-1.011949
1	2.165094	-1.969769	1.941814
8	1.792375	-0.069088	2.627002

$E_{(MeCN)}$ = -1248.916575
NImag = 1 (-193.6)

6. **1a**- A-$t^{‡}$ conformer 2 (-1248.686534)

6	1.742716	-3.332813	-0.337647
16	2.223451	-1.727856	-1.050065
6	2.732332	-0.759978	0.428094
6	3.754525	-2.231242	-1.932809
6	1.562082	-0.674541	1.764961
6	0.313141	-0.016865	1.224549
1	2.503770	-3.680422	0.365613
1	0.791550	-3.194039	0.176599
1	4.438256	-2.728247	-1.239947
1	4.209410	-1.317634	-2.320681
1	3.536678	-1.334337	0.899337
1	3.486252	-2.895684	-2.759552
1	1.621415	-4.039604	-1.162458
6	3.206494	0.594815	-0.002592
6	2.587267	1.347951	-1.017928
6	3.026607	2.638244	-1.321512
6	4.079531	3.211928	-0.602793
6	4.686579	2.482461	0.422640
6	4.260172	1.185636	0.716461
1	1.744171	0.937883	-1.569561
1	2.535557	3.199177	-2.113073
1	4.417013	4.218692	-0.835274
1	5.494141	2.923673	1.001418

1	4.718442	0.632603	1.530155
1	0.408018	1.044777	0.994583
6	-0.887146	-0.628140	1.127325
6	-2.109306	0.012129	0.680184
1	-0.970592	-1.676962	1.426587
1	-2.024022	1.065670	0.413591
6	-3.304441	-0.616514	0.581489
1	-3.345273	-1.670047	0.864009
6	-4.580545	-0.051064	0.134133
6	-5.716213	-0.884722	0.088115
6	-6.956625	-0.403454	-0.332824
6	-7.096293	0.931596	-0.720142
6	-5.980013	1.776282	-0.679034
6	-4.742311	1.294462	-0.259022
1	-5.618622	-1.925712	0.390049
1	-7.814190	-1.071632	-0.356457
1	-8.060446	1.311808	-1.047612
1	-6.076616	2.818240	-0.974930
1	-3.893549	1.972026	-0.233010
1	1.358717	-1.766330	1.923918
8	2.186672	-0.054403	2.707231

$E_{(MeCN)}$ = -1248.916190
NImag = 1 (-190.0)

7. **1a**-*c* conformer 1 (-1248.713880)

6	2.557514	-3.252886	0.959816
16	3.282810	-1.956434	-0.100746
6	2.307364	-0.351395	0.124057
6	4.714293	-1.575509	1.044785
6	1.280018	-0.671470	-1.019652
6	-0.034123	0.034182	-0.767296
1	1.952259	-2.784820	1.739802
1	1.917607	-3.852703	0.316667
1	4.379447	-1.338021	2.059953
1	5.272293	-0.730495	0.637444
1	1.811129	-0.470232	1.093673
1	5.361729	-2.457045	1.064556
1	3.369449	-3.836472	1.404093
6	3.120916	0.908787	0.095721
6	3.864872	1.273593	-1.040836
6	4.580876	2.471300	-1.069576
6	4.557814	3.331837	0.033072
6	3.816051	2.985722	1.165431
6	3.108560	1.781354	1.195938
1	3.882358	0.617253	-1.907421
1	5.152388	2.736276	-1.955405
1	5.111766	4.266652	0.007471
1	3.788455	3.650571	2.024993
1	2.529679	1.518822	2.078945
1	-0.011639	1.126901	-0.765867
6	-1.198657	-0.621058	-0.594753
6	-2.478934	0.026111	-0.384612
1	-1.170302	-1.709633	-0.630472
1	-2.472112	1.116568	-0.364149
6	-3.643543	-0.645506	-0.224353
1	-3.602841	-1.735254	-0.254341
6	-4.980957	-0.083697	-0.013963
6	-6.072409	-0.962492	0.138837
6	-7.368516	-0.486137	0.340558
6	-7.610188	0.888886	0.394920
6	-6.538800	1.778201	0.244735
6	-5.245524	1.301171	0.043573
1	-5.894660	-2.035231	0.096821
1	-8.189600	-1.189959	0.454261
1	-8.618008	1.265039	0.550778
1	-6.714257	2.850795	0.283529
1	-4.432571	2.012500	-0.072029
1	1.697488	-0.230050	-1.957282
8	1.241902	-2.034311	-1.036562

$E_{(MeCN)}$ = -1248.934253
NImag = 0

8. **1a**-*c* conformer 2 (-1248.713089)

6	4.038145	-3.005429	0.699354
16	3.920614	-1.496230	-0.321402
6	2.432837	-0.458457	0.230708
6	5.257706	-0.566388	0.608610
6	1.429453	-1.154022	-0.748503
6	0.036578	-1.181455	-0.171894
1	3.495945	-2.853405	1.636126
1	3.563231	-3.800440	0.128885
1	5.055230	-0.513753	1.683550
1	5.329681	0.443651	0.201383
1	2.234399	-0.797712	1.254481
1	6.201761	-1.091152	0.434750
1	5.094058	-3.209032	0.901791
6	2.634532	1.027662	0.197013
6	2.921716	1.696214	-1.006121
6	3.069635	3.083750	-1.032706
6	2.921633	3.829729	0.141394
6	2.627694	3.178789	1.342119
6	2.490401	1.788728	1.367563
1	3.031636	1.126969	-1.925913
1	3.293831	3.583959	-1.971366
1	3.030527	4.910937	0.118445
1	2.504497	3.750907	2.258122
1	2.256289	1.288156	2.304761
1	-0.082096	-1.813606	0.710922

6	-1.034435	-0.556438	-0.701291
6	-2.379022	-0.633072	-0.164056
1	-0.900728	0.046500	-1.601599
1	-2.506002	-1.255574	0.721803
6	-3.442296	0.013298	-0.696908
1	-3.266926	0.626498	-1.582253
6	-4.829976	-0.002376	-0.225514
6	-5.790402	0.766889	-0.912845
6	-7.126202	0.793399	-0.510101
6	-7.540205	0.046596	0.595715
6	-6.601003	-0.725646	1.290563
6	-5.267788	-0.750844	0.887596
1	-5.477910	1.351391	-1.775907
1	-7.843330	1.397026	-1.061218
1	-8.579688	0.062806	0.912952
1	-6.911717	-1.313211	2.151302
1	-4.560348	-1.361011	1.442074
1	1.398792	-0.556258	-1.685471
8	1.976881	-2.403693	-0.907420

$E_{(MeCN)}$ = -1248.933036
NImag = 0

9. **1a**-R‡ (-1248.701263) [$PCM_{(MeCN)}$/B3LYP/6-31+G* geometry]

6	-3.139328	-1.320915	-0.650588
6	-3.547712	-0.292467	0.219277
6	-4.924518	-0.050142	0.370843
6	-5.871489	-0.806693	-0.327899
6	-5.451804	-1.815896	-1.199394
6	-4.083636	-2.070041	-1.356831
6	-2.567564	0.554780	0.979044
6	-1.393253	-0.245274	1.849750
8	-1.558860	-1.570036	1.810840
6	-0.001487	0.273948	1.486756
6	0.999681	-0.504507	1.025038
6	2.344267	-0.032548	0.747792
6	3.334021	-0.830019	0.275859
6	4.716509	-0.449110	-0.035216
6	5.596322	-1.435355	-0.529761
6	6.923371	-1.132754	-0.845542
6	7.407292	0.168429	-0.673354
6	6.547596	1.161078	-0.181795
6	5.222700	0.858973	0.132756
16	-1.848008	1.941955	-0.100442
6	-3.308647	2.800626	-0.775386
6	-1.209839	1.166345	-1.617533
1	-3.116154	1.186746	1.691499
1	-1.587239	0.196642	2.861286
1	-2.943431	3.572019	-1.459808
1	-3.830372	3.268649	0.063198
1	-3.962605	2.095487	-1.292906
1	-1.994371	0.589876	-2.111348
1	-0.861667	1.980191	-2.260133
1	-0.372696	0.528178	-1.332444
1	0.789045	-1.562694	0.856567
1	-5.260882	0.730355	1.054510
1	-6.933344	-0.603726	-0.191449
1	-6.184928	-2.405744	-1.749181
1	-3.749799	-2.863780	-2.024776
1	-2.084605	-1.554166	-0.748384
1	2.535833	1.025815	0.940832
1	0.204584	1.328206	1.702024
1	3.096239	-1.882439	0.098385
1	4.577909	1.649379	0.513483
1	6.913812	2.178236	-0.042654
1	8.441384	0.408927	-0.918114
1	7.579666	-1.915226	-1.226255
1	5.227734	-2.452684	-0.666892

$E_{(MeCN)}$ = -1248.914144
NImag = 1 (-31.8)

10. **1a**-R‡ (-1242.405032) [HF/6-31+G* geometry]

6	5.413220	-1.437189	-0.597958
6	4.660720	-0.455703	0.046716
6	5.265048	0.781766	0.283942
6	6.562226	1.030597	-0.130306
6	7.293933	0.047339	-0.784566
6	6.713463	-1.189995	-1.013365
6	3.275506	-0.769329	0.454765
6	2.316663	0.101307	0.766209
6	0.961270	-0.290327	1.158046
6	-0.014989	0.567954	1.429756
6	-1.394597	0.108211	1.911523
8	-1.540962	-1.165018	2.056986
6	-2.609509	0.704663	0.912233
6	-3.464600	-0.322715	0.217900
6	-4.848628	-0.180936	0.219889
6	-5.669085	-1.109558	-0.408608
6	-5.106102	-2.199492	-1.049879
6	-3.725926	-2.362485	-1.042917
6	-2.911598	-1.441420	-0.406096
16	-2.002094	2.009749	-0.296383
6	-1.255512	1.153325	-1.696652
6	-3.474647	2.700504	-1.075942
1	-3.246476	1.329231	1.528175

1	-1.593441	0.716020	2.815776
1	-3.153006	3.415963	-1.821564
1	-4.045507	3.213085	-0.314346
1	-4.069992	1.920581	-1.526532
1	-1.971381	0.484502	-2.149326
1	-0.936225	1.909976	-2.401132
1	-0.401573	0.606237	-1.330044
1	0.738614	-1.339844	1.250063
1	-5.300492	0.649718	0.736035
1	-6.737112	-0.984036	-0.384904
1	-5.733894	-2.926336	-1.534285
1	-3.285340	-3.225328	-1.509985
1	-1.855820	-1.610104	-0.343917
1	2.518117	1.160229	0.727935
1	0.195266	1.631083	1.408747
1	3.033919	-1.819913	0.481876
1	4.728684	1.549276	0.811248
1	7.008041	1.989630	0.067426
1	8.303169	0.242019	-1.101092
1	7.270135	-1.963978	-1.511735
1	4.974378	-2.402946	-0.780317

$E_{(MeCN)}$ = -1248.910482
NImag = 1 (-37.1)

11. **1a**-*t* (-1242.412850) [HF/6-31+G* geometry]

6	3.741229	-3.124008	-0.223166
16	3.251711	-1.541748	-0.939701
6	2.826049	-0.480159	0.561121
6	4.850324	-0.903234	-1.482316
6	1.660872	-1.074458	1.489848
6	0.344303	-1.170807	0.728939
1	4.393943	-2.966085	0.623950
1	2.849649	-3.643001	0.091606
1	5.542659	-0.879738	-0.652057
1	4.692898	0.095339	-1.861113
1	3.718076	-0.552492	1.166623
1	5.225059	-1.540826	-2.271787
1	4.244289	-3.696380	-0.991033
6	2.646235	0.939282	0.079744
6	1.812457	1.278704	-0.982424
6	1.669058	2.601643	-1.374243
6	2.345598	3.606212	-0.699207
6	3.164277	3.279372	0.371453
6	3.315728	1.955451	0.754263
1	1.252255	0.520431	-1.498583
1	1.016809	2.845205	-2.193929
1	2.227216	4.632751	-0.997408
1	3.677732	4.052528	0.914701
1	3.925742	1.711369	1.604270
1	0.303865	-1.811388	-0.147113
6	-0.757774	-0.556358	1.136575
6	-2.054251	-0.661363	0.465483
1	-0.684914	0.053945	2.020080
1	-2.092609	-1.292835	-0.408131
6	-3.148439	-0.018865	0.869586
1	-3.067860	0.626844	1.729246
6	-4.487103	-0.067759	0.245813
6	-5.411455	0.931300	0.550924
6	-6.677289	0.938898	-0.016422
6	-7.050780	-0.061413	-0.899783
6	-6.146233	-1.071343	-1.203119
6	-4.883800	-1.077498	-0.635214
1	-5.133706	1.714297	1.235151
1	-7.368579	1.724449	0.233576
1	-8.032406	-0.061337	-1.339346
1	-6.429586	-1.861646	-1.876152
1	-4.210795	-1.882730	-0.866530
1	1.973992	-2.127686	1.665192
8	1.674358	-0.321828	2.553359

$E_{(MeCN)}$ = -1248.915608
NImag = 0

12. **1a**-$E^{\ddagger}$ conformer 1 (-1248.704660) [$PCM_{(MeCN)}$/6-31+G* geometry]

6	-4.950065	-0.647391	-1.031201
6	-4.694033	0.013642	0.190673
6	-5.769407	0.681829	0.813643
6	-7.045946	0.691907	0.245666
6	-7.281182	0.031596	-0.964911
6	-6.224289	-0.637404	-1.598486
6	-3.377199	0.041020	0.838116
6	-2.233640	-0.544831	0.406609
6	-0.971926	-0.460918	1.120361
6	0.174059	-1.035021	0.703315
6	1.463097	-1.024021	1.498003
8	1.508141	-0.250041	2.626728
6	2.702781	-0.428017	0.848637
16	3.213555	-1.765086	-0.977790
6	4.769052	-1.023046	-1.570068
6	3.851042	-3.272287	-0.171706
6	2.781896	0.936071	0.284694
6	1.778374	1.489132	-0.535001
6	1.921685	2.773457	-1.061161
6	3.068293	3.528255	-0.782127
6	4.076947	2.988403	0.023092
6	3.936615	1.700773	0.544213
1	4.533859	-3.013146	0.643154
1	2.993862	-3.823962	0.221908

1	5.461995	-0.862865	-0.739040
1	4.520193	-0.067474	-2.036151
1	3.598778	-0.717008	1.400559
1	5.216343	-1.688025	-2.314604
1	4.366779	-3.884978	-0.916882
1	0.887828	0.912845	-0.760774
1	1.136476	3.187305	-1.693185
1	3.175177	4.531515	-1.194033
1	4.972446	3.568335	0.244246
1	4.721788	1.284361	1.176082
1	0.177184	-1.620131	-0.222216
1	-0.955533	0.108025	2.052103
1	-2.227107	-1.119851	-0.522857
1	-3.337031	0.603732	1.774816
1	-5.595442	1.199702	1.757597
1	-7.857198	1.216660	0.750099
1	-8.274808	0.036696	-1.411829
1	-6.395650	-1.155037	-2.542302
1	-4.148073	-1.174271	-1.545675
1	1.689202	-2.099617	1.695613

$E_{(MeCN)}$ = -1248.917672
NImag = 1 (-236.1)

13. **1a**-$E^{‡}$ conformer 1 (-1242.407671) [HF/6-31+G* geometry]

6	4.208404	1.350330	0.240935
6	2.941671	0.771509	0.223391
6	1.926077	1.412906	-0.483787
6	2.182499	2.588318	-1.169537
6	3.453941	3.147289	-1.157058
6	4.468382	2.527875	-0.445243
6	2.724704	-0.495469	0.984988
6	1.448737	-0.779023	1.828527
6	0.161783	-0.989215	1.039751
6	-0.920048	-0.247078	1.237213
6	-2.207308	-0.470134	0.576851
16	3.049496	-2.115143	-0.344295
6	2.403075	-1.631921	-1.957861
6	4.823866	-2.094590	-0.673356
8	1.488122	0.244498	2.650037
1	1.652231	-1.765106	2.292836
1	5.133965	-1.120509	-1.024585
1	5.334344	-2.335516	0.248992
1	2.831190	-0.691704	-2.272600
1	1.331199	-1.533228	-1.870972
1	3.572922	-0.718343	1.610317
1	2.635370	-2.413697	-2.668979
1	5.055894	-2.850048	-1.412443
1	0.107206	-1.844914	0.375694
1	-0.839017	0.568190	1.936106
1	0.933352	1.010318	-0.474052
1	1.385328	3.077037	-1.700613
1	3.645818	4.064618	-1.684669
1	5.450489	2.964363	-0.408239
1	4.993301	0.896672	0.821056
1	-2.263720	-1.316558	-0.088781
6	-3.275008	0.301988	0.771379
1	-3.180834	1.123742	1.462925
6	-4.611303	0.158626	0.157944
6	-5.655195	0.951208	0.634131
6	-6.933121	0.856984	0.101820
6	-7.194749	-0.033658	-0.926218
6	-6.163622	-0.825903	-1.416866
6	-4.890072	-0.729932	-0.884802
1	-5.466268	1.646127	1.433883
1	-7.719747	1.478657	0.491673
1	-8.183339	-0.109898	-1.342769
1	-6.353175	-1.517423	-2.219088
1	-4.109700	-1.347133	-1.290489

$E_{(MeCN)}$ = -1248.913764
NImag = 1 (-276.8)

14. **1a**-$E^{‡}$ conformer 2 (-1242.410274) [HF/6-31+G* geometry]

6	-4.964065	-1.048113	-0.671040
6	-4.565769	-0.057585	0.230666
6	-5.487256	0.937621	0.555759
6	-6.752715	0.960222	-0.012073
6	-7.128027	-0.020999	-0.915746
6	-6.226113	-1.027037	-1.239307
6	-3.227329	-0.024692	0.856008
6	-2.135252	-0.664624	0.442599
6	-0.839900	-0.574342	1.118546
6	0.260608	-1.185615	0.702191
6	1.568273	-1.114965	1.468981
8	1.602625	-0.341670	2.536674
6	2.738168	-0.448031	0.711640
16	3.340682	-1.592640	-0.992553
6	4.908496	-0.834625	-1.470284
6	3.919142	-3.132549	-0.246441
6	2.636353	0.948974	0.183025
6	1.751852	1.308512	-0.830593
6	1.699306	2.616578	-1.285592
6	2.521668	3.584407	-0.725941
6	3.399433	3.237519	0.289645
6	3.458815	1.925777	0.735427
1	4.540942	-2.928615	0.615017

1	3.053242	-3.700165	0.059845
1	5.555589	-0.726317	-0.610016
1	4.690156	0.138553	-1.884444
1	3.637357	-0.603627	1.280642
1	5.386789	-1.449113	-2.221476
1	4.475651	-3.696345	-0.983406
1	1.095968	0.575513	-1.259809
1	1.008617	2.880656	-2.066277
1	2.472917	4.600687	-1.074556
1	4.029465	3.983926	0.739312
1	4.121269	1.665823	1.541144
1	0.227471	-1.812126	-0.181992
1	-0.769827	0.023606	2.010712
1	-2.173444	-1.281931	-0.440862
1	-3.145374	0.605757	1.726860
1	-5.207889	1.705698	1.256000
1	-7.442131	1.742294	0.253408
1	-8.109299	-0.009337	-1.355886
1	-6.511097	-1.802466	-1.928720
1	-4.292922	-1.849957	-0.918814
1	1.870497	-2.165515	1.645954

$E_{(MeCN)}$ = -1248.913341
NImag = 1 (-337.5)

15. **1a**-PC (-1248.757881)

6	4.464692	0.472084	0.242517
6	3.681593	-0.692988	0.244344
6	2.897444	-0.983401	1.368235
6	2.885651	-0.115399	2.463591
6	3.655535	1.050720	2.449348
6	4.447934	1.342102	1.333941
6	3.729268	-1.590472	-0.945622
6	2.578696	-1.853107	-1.869048
6	1.229020	-1.262360	-1.734235
6	0.268140	-1.706499	-0.898495
6	-1.053956	-1.121766	-0.797933
16	-0.915103	3.045045	-1.065486
6	-0.867956	2.695554	0.727442
6	0.860341	3.360662	-1.359139
8	3.008006	-2.828388	-0.910659
1	2.865458	-2.099300	-2.896454
1	1.465756	2.486387	-1.098863
1	0.980209	3.572900	-2.425525
1	-0.225521	1.836531	0.944958
1	-1.889323	2.458226	1.037521
1	4.719445	-1.679631	-1.399361
1	-0.520842	3.569588	1.288375
1	1.206012	4.228557	-0.787736
1	1.021368	-0.427823	-2.405507
1	0.485826	-2.564527	-0.263287
1	2.312969	-1.896890	1.384231
1	2.277047	-0.355034	3.332063
1	3.646884	1.722769	3.303752
1	5.059052	2.241164	1.317706
1	5.092680	0.697279	-0.617729
1	-1.244965	-0.246370	-1.417619
6	-2.018962	-1.604842	0.019553
1	-1.778812	-2.481852	0.622934
6	-3.379303	-1.088971	0.196065
6	-4.250244	-1.756275	1.080260
6	-5.556674	-1.310970	1.286395
6	-6.026156	-0.181571	0.611158
6	-5.174226	0.495210	-0.270770
6	-3.870040	0.050603	-0.476371
1	-3.892961	-2.637464	1.609396
1	-6.207040	-1.846528	1.973624
1	-7.042983	0.168925	0.768007
1	-5.529563	1.375204	-0.801419
1	-3.227876	0.594388	-1.163448

$E_{(MeCN)}$ = -1248.962773
NImag = 0

16. **1b**-A-$c^{\ddagger}$ conformer 1 (-1248.699399)

6	4.685535	1.361334	0.304778
6	4.591816	0.030950	-0.156329
6	5.776625	-0.731998	-0.191408
6	6.999562	-0.197104	0.215493
6	7.071716	1.121936	0.670306
6	5.905690	1.896544	0.711300
6	3.338270	-0.589080	-0.594081
6	2.106254	-0.027733	-0.637672
6	0.919752	-0.724674	-1.090493
6	-0.311728	-0.175845	-1.161216
6	-1.509760	-0.933936	-1.680137
8	-1.382174	-2.174585	-1.987491
6	-2.811725	-0.737325	-0.324604
6	-3.340529	0.638447	-0.131251
6	-2.717697	1.613212	0.676413
6	-3.217440	2.914371	0.748384
6	-4.342615	3.285929	0.005940
6	-4.965030	2.335203	-0.808048
6	-4.475649	1.029718	-0.870382
16	-2.158201	-1.441197	1.199571
6	-3.597202	-1.753286	2.296243
6	-1.701907	-3.137341	0.714942
1	-2.089285	-0.286954	-2.379650
1	-2.602804	-3.751622	0.642568
1	-1.240118	-3.041985	-0.284830

1	-4.349519	-2.339221	1.762089
1	-4.006539	-0.783555	2.587511
1	-3.558597	-1.426895	-0.725233
1	-3.243039	-2.291923	3.180456
1	-1.018146	-3.524061	1.473548
1	-1.828072	1.358831	1.248114
1	-2.718595	3.643314	1.382614
1	-4.726685	4.300980	0.060071
1	-5.839808	2.607186	-1.393719
1	-4.973318	0.299293	-1.504588
1	-0.461648	0.870247	-0.889461
1	1.028211	-1.758556	-1.419340
1	1.969056	1.008138	-0.325098
1	3.429402	-1.625415	-0.922641
1	5.730837	-1.759953	-0.545256
1	7.895972	-0.811090	0.176230
1	8.021871	1.543596	0.987831
1	5.949578	2.925240	1.061566
1	3.796218	1.984293	0.344932

$E_{(MeCN)}$ = -1248.923004
NImag = 1 (-190.4)

17. **1b**-A-$c^{‡}$ conformer 2 (-1248.698061)

6	4.977823	-0.277389	-1.144683
6	4.539753	-0.319508	0.196165
6	5.481334	-0.012888	1.199460
6	6.798084	0.324356	0.883895
6	7.212177	0.362664	-0.450005
6	6.292128	0.058533	-1.461150
6	3.171565	-0.663932	0.591514
6	2.122931	-0.948886	-0.217065
6	0.801036	-1.282748	0.269006
6	-0.248522	-1.583252	-0.523116
6	-1.592841	-1.968257	0.022704
6	-2.647081	-0.508153	-0.804579
6	-2.314100	0.841736	-0.278609
6	-2.223916	1.092536	1.105695
6	-1.866552	2.358477	1.576764
6	-1.580325	3.396022	0.684890
6	-1.643131	3.154956	-0.691098
6	-2.009199	1.893933	-1.164628
16	-4.352172	-1.054466	-0.632083
6	-4.635832	-1.330155	1.149669
6	-5.481806	0.364396	-0.920851
8	-1.783092	-2.028428	1.281949
1	-2.051326	-2.760819	-0.617551
1	-5.155556	1.221342	-0.326822
1	-5.449103	0.606951	-1.985306
1	-4.721315	-0.373683	1.670670
1	-3.751709	-1.883334	1.503847
1	-2.467718	-0.604413	-1.879709
1	-5.557919	-1.909231	1.241409
1	-6.493097	0.055686	-0.639399
1	-2.368956	0.272287	1.800494
1	-1.791832	2.527806	2.648401
1	-1.298238	4.377758	1.056779
1	-1.408189	3.948641	-1.396342
1	-2.052458	1.715523	-2.237709
1	-0.135691	-1.591663	-1.609521
1	0.640188	-1.308034	1.346341
1	2.251101	-0.934735	-1.300003
1	2.995671	-0.685172	1.667821
1	5.168558	-0.040209	2.241290
1	7.500642	0.556361	1.680760
1	8.237031	0.623843	-0.700935
1	6.603207	0.082031	-2.502983
1	4.285031	-0.512701	-1.947660

$E_{(MeCN)}$ = -1248.920963
NImag = 1 (-223.2)

18. **1b**-A-$c^{‡}$ conformer 3 (-1248.696842)

6	-3.860687	-2.807801	0.437874
16	-3.119151	-1.268722	1.071344
6	-2.935234	-0.270027	-0.421823
6	-4.513971	-0.558962	2.030737
6	-1.842291	-1.198569	-1.633592
1	-1.821853	-0.344236	-2.348127
8	-2.435155	-2.281360	-2.010492
6	-0.500245	-1.358146	-0.968104
1	-4.908111	-2.630958	0.180175
1	-3.284652	-3.042703	-0.476418
1	-5.389901	-0.454086	1.385541
1	-4.196145	0.417652	2.401552
1	-3.880989	-0.322883	-0.968498
1	-4.726823	-1.228692	2.869477
1	-3.768383	-3.567811	1.217036
6	-2.528007	1.126508	-0.116221
6	-1.504638	1.455118	0.796581
6	-1.109207	2.780505	0.984078
6	-1.710043	3.811637	0.255158
6	-2.715742	3.500793	-0.664690
6	-3.123197	2.177717	-0.842546
1	-0.998273	0.669850	1.351135
1	-0.317407	3.005354	1.694512
1	-1.395940	4.841915	0.399877
1	-3.190912	4.290343	-1.241852
1	-3.910817	1.949654	-1.557664
1	-0.391990	-2.258383	-0.358586

6	0.565099	-0.552771	-1.163354
6	1.873163	-0.767741	-0.577239
1	0.453932	0.319861	-1.809656
1	1.978048	-1.656004	0.046312
6	2.930467	0.058023	-0.761720
1	2.779646	0.936607	-1.390757
6	4.280442	-0.079482	-0.207879
6	5.234403	0.921218	-0.482153
6	6.533937	0.845446	0.020753
6	6.917197	-0.239134	0.813796
6	5.984436	-1.245230	1.094698
6	4.687386	-1.167987	0.592648
1	4.945712	1.769379	-1.099712
1	7.247274	1.633416	-0.208560
1	7.928691	-0.303585	1.206395
1	6.272196	-2.096505	1.707216
1	3.984748	-1.964445	0.821015

$E_{(MeCN)}$ = -1248.919795
NImag = 1 (-200.1)

19. **1b**-A-$t^{\ddagger}$ (-1248.686381)

6	0.587286	2.176543	-1.031925
16	2.007324	1.807610	0.047818
6	2.358390	0.031552	-0.375859
6	3.273483	2.879080	-0.752205
6	1.287871	-1.270562	0.267850
6	-0.060041	-0.661214	0.603663
1	0.872178	2.031427	-2.077300
1	-0.211318	1.483605	-0.762278
1	3.350178	2.631566	-1.813833
1	4.223151	2.682807	-0.251787
1	2.156450	-0.053916	-1.446882
1	2.983640	3.925091	-0.614609
1	0.279515	3.209483	-0.852789
6	3.784011	-0.275081	-0.038443
6	4.315903	-0.027664	1.241732
6	5.628856	-0.384346	1.553152
6	6.431484	-1.017655	0.598335
6	5.906759	-1.291481	-0.667107
6	4.598702	-0.917254	-0.985502
1	3.694682	0.431512	2.008812
1	6.019666	-0.182042	2.547376
1	7.450790	-1.304358	0.843583
1	6.514817	-1.800330	-1.410896
1	4.189507	-1.149436	-1.964667
1	-0.093540	0.031779	1.452590
6	-1.201716	-1.020537	-0.020200
6	-2.519873	-0.521974	0.317244
1	-1.113492	-1.748087	-0.827572
1	-2.576943	0.164540	1.163630
6	-3.649422	-0.863326	-0.348599
1	-3.547775	-1.550903	-1.189276
6	-5.018458	-0.416235	-0.077209
6	-6.054694	-0.836045	-0.935807
6	-7.376819	-0.440632	-0.728502
6	-7.700909	0.387179	0.349516
6	-6.685979	0.811206	1.216433
6	-5.366519	0.416272	1.007952
1	-5.812681	-1.482927	-1.776649
1	-8.153943	-0.781457	-1.408421
1	-8.729581	0.695920	0.516545
1	-6.926980	1.450321	2.062770
1	-4.599692	0.751197	1.700982
1	1.823334	-1.453043	1.234747
8	1.357622	-2.181434	-0.633285

$E_{(MeCN)}$ = -1248.916215
NImag = 1 (-221.9)

20. **1b**-*c* (-1248.700308)

6	-1.695616	-3.159488	0.714195
16	-2.176152	-1.458822	1.168192
6	-2.748655	-0.726453	-0.429086
6	-3.722149	-1.723242	2.105431
6	-1.521221	-0.866546	-1.557548
1	-1.976297	-0.222997	-2.357487
8	-1.340953	-2.130707	-1.890506
6	-0.297858	-0.109549	-1.049668
1	-2.584615	-3.793923	0.680650
1	-1.269749	-3.043624	-0.310536
1	-4.433471	-2.292256	1.501445
1	-4.133981	-0.744069	2.358068
1	-3.506302	-1.412451	-0.819249
1	-3.470204	-2.270289	3.018267
1	-0.981922	-3.508845	1.463473
6	-3.332488	0.636450	-0.182381
6	-2.727616	1.609687	0.635171
6	-3.281354	2.885512	0.758984
6	-4.443514	3.223817	0.059350
6	-5.050760	2.270115	-0.761827
6	-4.505245	0.989736	-0.874574
1	-1.813623	1.375969	1.175333
1	-2.797220	3.619265	1.398646
1	-4.869247	4.219337	0.152337
1	-5.953711	2.519460	-1.313431
1	-4.986593	0.254791	-1.516003
1	-0.422004	0.941940	-0.782297
6	0.927454	-0.671960	-1.007753
6	2.134040	0.011143	-0.585268
1	1.008229	-1.707929	-1.337635

1	2.019908	1.052189	-0.279901
6	3.357324	-0.569439	-0.557284
1	3.425766	-1.610456	-0.876289
6	4.628031	0.034506	-0.146583
6	5.798270	-0.750628	-0.183991
6	7.036123	-0.232224	0.198581
6	7.138985	1.092536	0.630396
6	5.988049	1.889361	0.672698
6	4.753014	1.370412	0.290560
1	5.728988	-1.783222	-0.520220
1	7.920465	-0.863702	0.158002
1	8.100933	1.501391	0.928667
1	6.055498	2.922892	1.004459
1	3.876329	2.010856	0.330252

$E_{(MeCN)}$ = -1248.927384
NImag = 0

21. **1b**-R‡ conformer 1 (-1248.683348)

6	-3.873720	2.352720	1.562133
16	-2.779780	2.148707	0.107187
6	-2.115867	0.389151	0.118362
6	-4.035676	2.140793	-1.211896
6	-1.121467	0.231247	-1.276530
1	-1.465430	1.097783	-1.931391
8	-1.245764	-0.948823	-1.794208
6	0.259771	0.654216	-0.780012
1	-4.577062	1.518942	1.621196
1	-3.237117	2.373765	2.449447
1	-4.770329	1.355330	-1.022386
1	-3.516514	1.957316	-2.153771
1	-1.466868	0.420235	1.001072
1	-4.503835	3.128058	-1.225848
1	-4.400268	3.306905	1.466511
6	-3.194936	-0.634075	0.299528
6	-3.891702	-1.170800	-0.799350
6	-4.895935	-2.121203	-0.600402
6	-5.212604	-2.562516	0.688222
6	-4.509303	-2.057500	1.785218
6	-3.508136	-1.103088	1.587664
1	-3.583472	-0.894040	-1.800905
1	-5.415687	-2.537530	-1.459660
1	-5.988822	-3.309552	0.834900
1	-4.730139	-2.411555	2.789072
1	-2.946323	-0.733095	2.443759
1	0.368380	1.677075	-0.402263
6	1.329937	-0.160824	-0.842393
6	2.666203	0.203577	-0.415599
1	1.166199	-1.157608	-1.251906
1	2.792889	1.218921	-0.036809
6	3.728711	-0.634681	-0.461688
1	3.556781	-1.642673	-0.841215
6	5.108120	-0.354458	-0.052859
6	6.064880	-1.387017	-0.129701
6	7.392541	-1.180217	0.247139
6	7.803807	0.071651	0.711862
6	6.868986	1.111316	0.792668
6	5.543827	0.903112	0.416710
1	5.755037	-2.365610	-0.490730
1	8.105963	-1.997909	0.176551
1	8.837065	0.238093	1.005522
1	7.177140	2.091623	1.149103
1	4.840375	1.728372	0.483975

$E_{(MeCN)}$ = -1248.917580
NImag = 1 (-36.1)

22. **1b**-R‡ conformer 1 (-1248.704334)

[$PCM_{(MeCN)}$/B3LYP/6-31+G* geometry]

6	4.171686	-1.969712	1.725150
16	3.080408	-2.140408	0.275766
6	2.155281	-0.501428	0.144095
6	4.304218	-2.124686	-1.070254
6	1.177320	-0.634449	-1.188295
1	1.452925	-1.637065	-1.623954
8	1.310086	0.366141	-2.059179
6	-0.218489	-0.864100	-0.609362
1	4.790968	-1.075098	1.632219
1	3.532866	-1.908229	2.609825
1	4.982390	-1.277007	-0.958045
1	3.759440	-2.067005	-2.015169
1	1.545485	-0.574092	1.054669
1	4.848447	-3.071376	-1.012083
1	4.788449	-2.871663	1.776276
6	3.046857	0.700457	0.254032
6	3.834782	1.165361	-0.815800
6	4.653616	2.286878	-0.657333
6	4.692940	2.970384	0.563770
6	3.904631	2.526697	1.630144
6	3.092455	1.399244	1.474442
1	3.773058	0.674333	-1.780430
1	5.255989	2.634657	-1.496280
1	5.329999	3.846855	0.680572
1	3.920987	3.053966	2.583552
1	2.477859	1.061554	2.309938
1	-0.326897	-1.721182	0.065377
6	-1.297543	-0.110036	-0.898845
6	-2.625662	-0.349319	-0.362080
1	-1.167695	0.732689	-1.580801
1	-2.727580	-1.209259	0.304551
6	-3.702720	0.424820	-0.641665

1	-3.555785	1.279907	-1.307170
6	-5.073477	0.258529	-0.143740
6	-6.049165	1.209479	-0.511144
6	-7.369468	1.106275	-0.065544
6	-7.751201	0.043825	0.760572
6	-6.795952	-0.912438	1.133350
6	-5.477863	-0.808744	0.688871
1	-5.761030	2.041330	-1.154969
1	-8.100492	1.857195	-0.365008
1	-8.779669	-0.041340	1.109938
1	-7.082041	-1.746230	1.774527
1	-4.758359	-1.567769	0.991452

$E_{(MeCN)}$ = -1248.917224
NImag = 1 (-23.4)

23. **1b**-R‡ conformer 1 (-1242.409874) [HF/6-31+G* geometry]

6	-3.839325	2.241773	1.668204
16	-2.809649	2.124428	0.192952
6	-2.103164	0.386326	0.131398
6	-4.057521	2.192398	-1.106285
6	-1.123559	0.346581	-1.195621
1	-1.430737	1.243700	-1.787469
8	-1.231261	-0.774695	-1.831495
6	0.265448	0.700899	-0.666870
1	-4.577675	1.454050	1.681570
1	-3.193171	2.161999	2.531248
1	-4.822627	1.451970	-0.929268
1	-3.565052	2.005858	-2.048293
1	-1.501129	0.384540	1.031617
1	-4.477058	3.189504	-1.102824
1	-4.315043	3.213705	1.668142
6	-3.176211	-0.662802	0.255069
6	-3.861716	-1.161970	-0.853073
6	-4.852661	-2.116973	-0.688718
6	-5.161174	-2.606805	0.573740
6	-4.465551	-2.141579	1.677691
6	-3.480172	-1.177660	1.513071
1	-3.569597	-0.847922	-1.834389
1	-5.364844	-2.501009	-1.552936
1	-5.921824	-3.358270	0.691171
1	-4.676017	-2.531744	2.657661
1	-2.928905	-0.841952	2.375591
1	0.384427	1.649650	-0.154704
6	1.315520	-0.088526	-0.847476
6	2.667263	0.222512	-0.379757
1	1.155761	-1.010695	-1.379069
1	2.790331	1.158667	0.141356
6	3.713198	-0.582603	-0.555741

1	3.549537	-1.524478	-1.054383
6	5.101684	-0.341832	-0.111020
6	5.981650	-1.420937	-0.027913
6	7.291755	-1.251060	0.395167
6	7.754987	0.008954	0.739051
6	6.894785	1.096107	0.648333
6	5.588035	0.924581	0.224818
1	5.634206	-2.405005	-0.291246
1	7.947268	-2.102114	0.454130
1	8.770950	0.145747	1.064530
1	7.246757	2.081669	0.898550
1	4.949290	1.784552	0.139354

$E_{(MeCN)}$ = -1248.914370
NImag = 1 (-36.6)

24. **1b**-R‡ conformer 2 (-1242.409648) [HF/6-31+G* geometry]

6	6.004655	1.065316	-0.028040
6	5.075476	0.027899	-0.104066
6	5.497758	-1.255200	0.254126
6	6.791122	-1.481607	0.692389
6	7.701207	-0.435174	0.775696
6	7.301683	0.840114	0.409415
6	3.703692	0.326553	-0.565285
6	2.621519	-0.430728	-0.396802
6	1.285739	-0.073892	-0.880121
6	0.202601	-0.821486	-0.696035
6	-1.194973	-0.517452	-1.219771
8	-1.773985	-1.514850	-1.810809
6	-2.047192	-0.018137	0.106392
6	-3.452135	-0.528836	0.291988
6	-3.908454	-0.808226	1.578369
6	-5.196238	-1.276326	1.799993
6	-6.047825	-1.475985	0.725501
6	-5.597900	-1.221960	-0.563416
6	-4.308771	-0.762516	-0.784349
16	-1.967615	1.849805	0.072868
6	-3.117042	2.354857	-1.220613
6	-2.814240	2.455751	1.544366
1	-1.474720	-0.223736	1.002946
1	-1.087188	0.399604	-1.842440
1	-2.849581	3.535850	1.488378
1	-2.230070	2.163713	2.405866
1	-3.809890	2.043297	1.610723
1	-4.114656	2.012036	-0.992269
1	-3.084687	3.434437	-1.281837
1	-2.777212	1.925811	-2.150976
1	1.208000	0.847930	-1.437595
1	-3.247977	-0.679394	2.419777

1	-5.523486	-1.493224	2.801375
1	-7.045263	-1.844755	0.887322
1	-6.243106	-1.408922	-1.403306
1	-3.938920	-0.646058	-1.782624
1	0.278153	-1.766308	-0.177398
1	2.694691	-1.367707	0.130487
1	3.590982	1.270587	-1.075389
1	4.820427	-2.085567	0.174673
1	7.093442	-2.478915	0.959738
1	8.706622	-0.615331	1.112388
1	7.996635	1.659775	0.461754
1	5.707436	2.061000	-0.309433

$E_{(MeCN)}$ = -1248.912755
NImag = 1 (-31.0)

25. **1b**-*t* conformer 1 (-1242.412322) [HF/6-31+G* geometry]

6	6.150661	-1.373790	0.176532
6	5.132015	-0.422190	0.128950
6	5.494540	0.925974	0.196023
6	6.823457	1.302289	0.286376
6	7.827314	0.342308	0.320798
6	7.483152	-0.998875	0.268065
6	3.731478	-0.880271	0.020232
6	2.673598	-0.150896	-0.329485
6	1.314511	-0.687735	-0.416463
6	0.252710	0.026140	-0.768822
6	-1.136278	-0.602745	-0.890273
8	-1.203119	-1.883837	-0.659950
6	-2.104184	0.067246	0.185460
6	-3.492574	-0.512075	0.268268
6	-4.124851	-0.623912	1.501697
6	-5.402431	-1.157721	1.607694
6	-6.063120	-1.593979	0.471499
6	-5.431979	-1.510224	-0.763202
6	-4.155711	-0.982502	-0.863500
16	-2.173413	1.968050	-0.053676
6	-3.133989	2.242977	-1.554054
6	-3.289395	2.634718	1.196172
1	-1.606512	0.007782	1.144278
1	-1.514082	-0.282751	-1.889753
1	-3.377122	3.700214	1.029235
1	-2.842443	2.462141	2.165099
1	-4.255827	2.157087	1.141303
1	-4.090648	1.746919	-1.486773
1	-3.263578	3.310734	-1.671033
1	-2.567702	1.854053	-2.386608
1	1.159276	-1.729689	-0.196224
1	-3.607872	-0.319707	2.396042
1	-5.867782	-1.245314	2.573394
1	-7.049328	-2.016314	0.547097
1	-5.923752	-1.881781	-1.644463
1	-3.655879	-0.982823	-1.812694
1	0.380352	1.069793	-1.030884
1	2.794907	0.891222	-0.578916
1	3.576310	-1.925980	0.232121
1	4.735913	1.687060	0.191139
1	7.077319	2.346671	0.338067
1	8.858953	0.637542	0.393845
1	8.248377	-1.754488	0.297970
1	5.897122	-2.418903	0.134357

$E_{(MeCN)}$ = -1248.918064
NImag = 0

26. **1b**-*t* conformer 2 (-1242.412830) [HF/6-31+G* geometry]

6	-5.886653	0.549861	1.134925
6	-5.003678	-0.144127	0.307991
6	-5.504035	-0.676001	-0.883377
6	-6.829543	-0.497220	-1.240005
6	-7.693531	0.208896	-0.412300
6	-7.215631	0.728942	0.779888
6	-3.595170	-0.294168	0.729031
6	-2.559914	-0.613585	-0.045029
6	-1.183610	-0.743942	0.438002
6	-0.144942	-1.053307	-0.331995
6	1.278171	-1.284660	0.158844
8	1.745834	-2.472477	-0.120996
6	2.253953	-0.269892	-0.583173
6	3.704802	-0.351757	-0.185825
6	4.691216	-0.292090	-1.164864
6	6.036271	-0.368364	-0.833154
6	6.414143	-0.509286	0.492596
6	5.438835	-0.590660	1.476852
6	4.096449	-0.519193	1.140199
16	1.603574	1.526888	-0.498111
6	1.557997	1.959140	1.250187
6	2.931157	2.604596	-1.074432
1	2.144845	-0.459504	-1.642304
1	1.286358	-1.007757	1.232606
1	2.590134	3.627156	-0.978116
1	3.108682	2.385825	-2.117739
1	3.834489	2.444988	-0.505578
1	2.516868	1.773685	1.710850
1	1.299058	3.007154	1.321989
1	0.789092	1.364565	1.717157
1	-1.034792	-0.607456	1.499501

1	4.408925	-0.212720	-2.200741
1	6.781336	-0.332527	-1.607923
1	7.454819	-0.576683	0.755197
1	5.721999	-0.734541	2.504303
1	3.356205	-0.641897	1.907701
1	-0.301069	-1.252523	-1.382902
1	-2.706070	-0.786089	-1.098606
1	-3.410880	-0.105546	1.775279
1	-4.862246	-1.248229	-1.527795
1	-7.192664	-0.919222	-2.160597
1	-8.723947	0.341918	-0.690098
1	-7.874193	1.271600	1.435061
1	-5.528513	0.958310	2.064344

$E_{(MeCN)}$ = -1248.917869
NImag = 0

27. **1b**-E‡ conformer 1 (-1242.411256) [HF/6-31+G* geometry]

6	-3.378184	2.469071	1.480390
16	-2.105151	1.974299	0.301152
6	-2.082536	-0.134345	0.202980
6	-2.866070	2.491009	-1.250516
6	-1.136105	-0.600289	-0.936855
6	0.247923	0.021605	-0.792304
1	-4.323351	2.002958	1.244189
1	-3.054833	2.163934	2.465838
1	-3.814597	1.993206	-1.391912
1	-2.190935	2.234756	-2.053604
1	-1.603286	-0.294174	1.154254
1	-3.004344	3.563972	-1.226983
1	-3.469590	3.547153	1.456519
6	-3.506694	-0.587527	0.186727
6	-4.198686	-0.794973	-1.005056
6	-5.517037	-1.217712	-0.987383
6	-6.162257	-1.452622	0.220180
6	-5.476810	-1.272794	1.410829
6	-4.156935	-0.845275	1.389259
1	-3.695911	-0.670035	-1.944608
1	-6.033921	-1.386911	-1.915023
1	-7.182808	-1.791678	0.229814
1	-5.958611	-1.477722	2.350160
1	-3.622613	-0.736159	2.317424
1	0.362482	1.081620	-0.983360
6	1.317416	-0.706998	-0.499408
6	2.673830	-0.167397	-0.388595
1	1.172299	-1.762314	-0.345628
1	2.783714	0.892483	-0.553602
6	3.738017	-0.909877	-0.090127
1	3.585829	-1.961131	0.095057
6	5.134672	-0.446755	0.045433
6	6.054578	-1.261410	0.705186
6	7.374939	-0.869293	0.870479
6	7.807337	0.348564	0.370503
6	6.906179	1.165428	-0.301084
6	5.589323	0.771953	-0.465490
1	5.731359	-2.209763	1.098347
1	8.062183	-1.515728	1.387403
1	8.830881	0.655191	0.493371
1	7.233565	2.106987	-0.706072
1	4.917360	1.410633	-1.008904
1	-1.537367	-0.229636	-1.900830
8	-1.210313	-1.901077	-0.758897

$E_{(MeCN)}$ = -1248.917275
NImag = 1 (-287.9)

28. **1b**-E‡ conformer 2 (-1242.412071) [HF/6-31+G* geometry]

6	-4.354838	-0.703310	1.288082
6	-3.662651	-0.467900	0.106247
6	-4.349905	-0.545765	-1.102719
6	-5.703239	-0.839428	-1.124626
6	-6.387352	-1.069306	0.062107
6	-5.709041	-1.005969	1.268880
6	-2.200581	-0.147983	0.156778
16	-2.075568	1.887634	-0.301771
6	-0.816384	2.477178	0.853038
6	-1.253719	-1.010841	-0.720568
8	-1.337156	-2.139793	-0.048902
6	0.136423	-0.400969	-0.852369
6	1.203534	-0.933698	-0.269801
6	2.565064	-0.413982	-0.413318
6	3.622468	-0.936001	0.205349
6	5.021835	-0.469608	0.115391
6	5.490914	0.340291	-0.922188
6	6.808903	0.762484	-0.954290
6	7.695881	0.379514	0.044058
6	7.249137	-0.436337	1.071311
6	5.927934	-0.857889	1.101967
6	-3.542855	2.687370	0.384386
1	-1.100376	2.235720	1.868541
1	0.113664	1.987015	0.610952
1	-3.689455	2.398056	1.415358
1	-4.396475	2.382401	-0.201386
1	-1.812854	-0.107001	1.159854
1	-3.414475	3.759304	0.308600
1	-0.709287	3.547616	0.740272
1	-3.828300	-0.391881	-2.029755
1	-6.220194	-0.902773	-2.065467

1	-7.435996	-1.307023	0.043033
1	-6.226413	-1.201906	2.191015
1	-3.827826	-0.682143	2.225553
1	0.254955	0.455801	-1.506584
1	1.052280	-1.813318	0.332221
1	2.686772	0.443485	-1.056356
1	3.461955	-1.777943	0.859593
1	5.593495	-1.492212	1.904627
1	7.926128	-0.747434	1.847334
1	8.720420	0.705247	0.014084
1	7.148438	1.382199	-1.765631
1	4.830406	0.627582	-1.719718
1	-1.669688	-1.031682	-1.742894

$E_{(MeCN)}$ = -1248.916627
NImag = 1 (-268.4)

29. **1b**-PC (-1248.761486)

6	5.576253	0.994321	0.339412
6	5.266986	-0.334591	-0.019561
6	6.334042	-1.248226	-0.131683
6	7.652942	-0.857261	0.102451
6	7.939645	0.463354	0.456813
6	6.892335	1.385762	0.573372
6	3.903908	-0.806096	-0.278384
6	2.756803	-0.088219	-0.233500
6	1.451043	-0.650958	-0.509500
6	0.301718	0.056316	-0.487723
6	-1.035501	-0.510420	-0.769027
8	-1.119402	-1.894747	-1.138188
6	-1.699734	-1.515555	0.117294
16	-2.740859	3.279316	-0.272163
6	-4.212189	2.872094	-1.276569
6	-3.429496	3.000389	1.397140
6	-3.179877	-1.612323	0.259876
6	-4.016106	-1.719290	-0.861221
6	-5.402363	-1.780447	-0.703307
6	-5.970698	-1.736713	0.574192
6	-5.142086	-1.639278	1.696120
6	-3.755180	-1.581765	1.538881
1	-3.754775	1.962682	1.523010
1	-2.632192	3.211459	2.115656
1	-4.528028	1.836342	-1.114158
1	-3.932238	2.997021	-2.326575
1	-1.122517	-1.841143	0.984522
1	-5.041961	3.550530	-1.051844
1	-4.267948	3.676562	1.594917
1	-3.570933	-1.775022	-1.850676
1	-6.040326	-1.871299	-1.579131
1	-7.049810	-1.788072	0.694761
1	-5.573797	-1.616876	2.693715
1	-3.113360	-1.516986	2.415591
1	0.312131	1.123388	-0.264949
1	1.404845	-1.710190	-0.762573
1	2.783484	0.971961	0.017945
1	3.825886	-1.862765	-0.538436
1	6.119714	-2.278711	-0.407670
1	8.455790	-1.584269	0.007790
1	8.965250	0.772930	0.640294
1	7.104513	2.416112	0.848519
1	4.781735	1.728737	0.436797
1	-1.711182	0.139967	-1.327857

$E_{(MeCN)}$ = -1248.967015
NImag = 0

1,4- Addition (Pathway 2)

30. **2a**-A-$c^{\ddagger}$ conformer 1 (-1248.691616)

6	1.034991	1.760740	-1.115363
6	0.910599	1.318093	0.220619
6	0.118325	2.098796	1.090474
6	-0.500519	3.271210	0.657211
6	-0.339780	3.708088	-0.661757
6	0.428653	2.943305	-1.544414
6	1.473418	0.032854	0.686004
16	3.247566	-0.160818	0.779643
6	3.962428	0.208740	-0.852434
6	0.687868	-1.687206	-0.278683
6	1.374775	-2.868925	0.094330
6	2.562037	-3.284243	-0.549773
8	3.197589	-2.639839	-1.422360
6	-0.713527	-1.550072	0.141313
6	-1.656273	-0.870857	-0.544153
6	-3.079521	-0.734714	-0.206850
6	-3.876844	0.140682	-0.969505
6	-5.233578	0.315457	-0.692112
6	-5.830592	-0.387566	0.357115
6	-5.055229	-1.268321	1.121323
6	-3.700867	-1.441022	0.843516
6	3.917148	1.280997	1.709588
1	3.559858	2.212891	1.264860
1	3.566807	1.196511	2.740588
1	3.708324	1.222151	-1.169248
1	3.590145	-0.572227	-1.521629
1	1.145366	-0.243839	1.690651
1	0.977516	-3.492435	0.893362
1	5.044394	0.096862	-0.741142
1	5.010043	1.231677	1.686313
1	2.957614	-4.274014	-0.239140
1	-0.977504	-2.066802	1.064433
1	-1.350250	-0.355219	-1.454552

1	0.917959	-1.297741	-1.268653
1	-3.123654	-2.141193	1.440884
1	-5.511737	-1.828432	1.933971
1	-6.887562	-0.257664	0.574968
1	-5.823789	0.999674	-1.296919
1	-3.419188	0.693583	-1.787085
1	-0.016928	1.770913	2.119038
1	-1.108591	3.845883	1.351701
1	-0.817527	4.623722	-1.000061
1	0.541989	3.256944	-2.579552
1	1.573876	1.154346	-1.836873

$E_{(MeCN)}$ = -1248.910869
NImag = 1 (-266.2)

31. **2a**-A-$c^{\ddagger}$ conformer 2 (-1248.688731)

6	-2.407746	1.534657	0.756716
6	-1.525858	1.230614	-0.306418
6	-0.874852	2.298893	-0.959984
6	-1.104512	3.621511	-0.578451
6	-2.002587	3.911921	0.454088
6	-2.649115	2.861992	1.115433
6	-1.211214	-0.160372	-0.677578
16	-2.650770	-1.176235	-0.956004
6	-3.591815	-0.431771	-2.348115
6	-0.296251	-1.103962	0.998829
6	-0.919392	-2.313025	1.410161
6	-2.115060	-2.309988	2.175588
8	-2.817963	-1.309993	2.443004
6	1.099116	-1.146095	0.543068
6	1.968806	-0.121132	0.669972
6	3.379601	-0.088474	0.263209
6	4.109824	1.102378	0.445136
6	5.451770	1.196125	0.072734
6	6.101426	0.095544	-0.491302
6	5.393032	-1.098318	-0.675670
6	4.053509	-1.189922	-0.304059
6	-1.924376	-2.603602	-1.814322
1	-1.356386	-2.266286	-2.686417
1	-1.280204	-3.103182	-1.090209
1	-2.947138	-0.301771	-3.220833
1	-3.953517	0.538029	-2.000194
1	-0.532447	-0.258102	-1.527909
1	-0.441941	-3.270156	1.199877
1	-4.440548	-1.083041	-2.578892
1	-2.735665	-3.271652	-2.113266
1	-2.438637	-3.304016	2.557389
1	1.426007	-2.084759	0.093275
1	1.602332	0.797642	1.128841
1	-0.567768	-0.227936	1.584199
1	3.528665	-2.130114	-0.449246
1	5.890271	-1.963343	-1.108162
1	7.146893	0.162906	-0.780923
1	5.989598	2.128639	0.225437
1	3.611902	1.963892	0.885160
1	-0.182903	2.084480	-1.772062
1	-0.587799	4.426857	-1.095497
1	-2.187120	4.942376	0.746783
1	-3.331012	3.073668	1.935571
1	-2.862406	0.723714	1.324908

$E_{(MeCN)}$ = -1248.910697
NImag = 1 (-279.8)

32. **2a**-A-$c^{\ddagger}$ conformer 3 (-1248.684396)

6	-3.644106	-1.663116	0.699826
6	-3.153206	-0.685143	-0.189073
6	-4.065740	0.265117	-0.686583
6	-5.408816	0.251403	-0.306257
6	-5.875875	-0.720777	0.581500
6	-4.984600	-1.678980	1.079790
6	-1.749398	-0.610723	-0.619534
6	-0.714191	-1.346316	-0.167413
6	0.670267	-1.243574	-0.669880
6	1.368263	0.174854	0.590452
16	3.163836	-0.049230	0.549320
6	3.483290	-1.478777	1.632833
6	0.956978	1.516775	0.140449
6	1.471562	2.110587	-1.035340
6	0.994788	3.341845	-1.487326
6	-0.021071	4.008160	-0.794473
6	-0.553688	3.425871	0.360960
6	-0.068865	2.203408	0.825265
6	3.857300	1.283215	1.598821
6	1.456321	-2.432105	-0.684817
6	2.582740	-2.596441	-1.525321
8	3.428352	-3.514393	-1.474884
1	2.906014	-1.378086	2.555604
1	3.204805	-2.375248	1.078760
1	3.425727	1.238067	2.601519
1	3.608128	2.234012	1.124417
1	1.008813	-0.091013	1.587317
1	1.239137	-3.223724	0.033442
1	4.943445	1.156766	1.635233
1	4.556048	-1.485413	1.842401
1	2.709809	-1.798219	-2.299153
1	-0.872123	-2.094170	0.610051
1	-1.547889	0.129579	-1.394049

1	0.774960	-0.606630	-1.551698
1	-2.975883	-2.426952	1.087691
1	-5.339186	-2.447123	1.762962
1	-6.921475	-0.738224	0.877921
1	-6.089982	0.998750	-0.705962
1	-3.710272	1.025482	-1.378897
1	-0.492603	1.764010	1.725058
1	-1.347334	3.928501	0.908445
1	-0.394065	4.964369	-1.151154
1	1.411966	3.776071	-2.392727
1	2.242042	1.600336	-1.610503

$E_{(MeCN)}$ = -1248.910493
NImag = 1 (-315.2)

33. **2a**-A-$t^{\ddagger}$ (-1248.692287)

6	0.267302	1.905256	-0.858272
6	1.306799	1.439269	-0.023576
6	1.770474	2.303593	0.990982
6	1.216896	3.574095	1.165362
6	0.200046	4.025637	0.319932
6	-0.267872	3.182260	-0.694782
6	1.848178	0.066404	-0.089511
16	2.149457	-0.491150	-1.760753
6	3.770881	0.218492	-2.285065
6	0.731648	-1.255878	1.067893
6	1.393562	-1.254442	2.324372
6	2.635616	-1.909876	2.480255
8	3.288017	-2.472998	1.560981
6	-0.654977	-0.779399	0.985327
6	-1.577282	-1.291179	0.144388
6	-2.987467	-0.902162	0.013855
6	-3.821153	-1.643330	-0.845943
6	-5.170054	-1.321879	-1.005990
6	-5.720235	-0.244384	-0.307710
6	-4.905381	0.506232	0.548910
6	-3.559043	0.184949	0.706734
6	2.655517	-2.235343	-1.539971
1	3.105875	-2.362808	-0.545163
1	1.761127	-2.855427	-1.626182
1	4.538057	-0.058152	-1.557318
1	3.646215	1.302760	-2.316699
1	2.765905	-0.082409	0.477403
1	0.988797	-0.682533	3.156202
1	4.020563	-0.160759	-3.280442
1	3.346719	-2.482413	-2.349371
1	3.069972	-1.901945	3.500887
1	-0.923540	0.023435	1.670407
1	-1.269137	-2.107628	-0.512287

1	0.945787	-2.121444	0.446022
1	-2.945013	0.786955	1.370159
1	-5.322587	1.348883	1.095024
1	-6.770085	0.010099	-0.428025
1	-5.790275	-1.914042	-1.674465
1	-3.401760	-2.486610	-1.391321
1	2.569793	1.968394	1.647136
1	1.592073	4.216394	1.958667
1	-0.222617	5.018698	0.447770
1	-1.064923	3.515350	-1.355266
1	-0.137128	1.257710	-1.632061

$E_{(MeCN)}$ = -1248.908761
NImag = 1 (-292.7)

34. **2a**-*c* conformer 1 (-1248.713544)

6	1.245799	1.595983	-1.177331
6	1.168471	1.156740	0.156090
6	0.848741	2.096490	1.149481
6	0.613522	3.435482	0.826778
6	0.698527	3.858861	-0.501502
6	1.014924	2.934042	-1.501626
6	1.362486	-0.293681	0.524720
16	3.199844	-0.818978	0.558515
6	4.114443	0.150469	-0.689982
6	0.484261	-1.319301	-0.271043
6	0.930491	-2.755777	-0.119287
6	2.066441	-3.131281	-0.787948
8	2.857355	-2.276020	-1.357902
6	-0.942104	-1.130558	0.187359
6	-1.938093	-0.659649	-0.580305
6	-3.353737	-0.489689	-0.210473
6	-4.210737	0.181448	-1.102597
6	-5.559710	0.381360	-0.803152
6	-6.087489	-0.092058	0.400256
6	-5.251510	-0.769854	1.295893
6	-3.905335	-0.968091	0.994573
6	3.702705	0.212781	2.014099
1	3.429968	1.265005	1.896662
1	3.222436	-0.207234	2.901912
1	3.871455	1.212773	-0.624786
1	3.857182	-0.281297	-1.655223
1	1.139826	-0.431599	1.589237
1	0.267407	-3.483683	0.338994
1	5.174967	-0.014644	-0.478863
1	4.786903	0.115840	2.121166
1	2.348583	-4.197850	-0.816655
1	-1.141820	-1.436112	1.216420
1	-1.695205	-0.356857	-1.599822

1	0.559414	-1.039951	-1.330587
1	-3.280134	-1.511616	1.697537
1	-5.653870	-1.152225	2.231016
1	-7.137756	0.057783	0.636922
1	-6.197609	0.904667	-1.511320
1	-3.808082	0.552817	-2.042780
1	0.758977	1.771780	2.184082
1	0.356625	4.142529	1.611319
1	0.512990	4.898745	-0.757332
1	1.076836	3.253078	-2.538948
1	1.482008	0.887558	-1.965973

$E_{(MeCN)}$ = -1248.935392
NImag = 0

35. **2a**-*c* conformer 2 (-1248.710025)

6	-2.387107	1.494780	0.925774
6	-1.685743	1.150249	-0.244439
6	-1.424628	2.138142	-1.205657
6	-1.855666	3.453390	-1.009365
6	-2.562607	3.788162	0.148275
6	-2.825871	2.806961	1.111245
6	-1.180297	-0.254123	-0.449044
16	-2.608739	-1.498405	-0.595744
6	-3.719134	-0.556501	-1.754274
6	-0.249364	-0.839590	0.683809
6	-0.722939	-2.208420	1.125762
6	-1.713239	-2.279159	2.116418
8	-2.414163	-1.308933	2.518989
6	1.176417	-0.836545	0.199611
6	2.132062	-0.007186	0.652700
6	3.545422	0.046981	0.242361
6	4.355600	1.085036	0.739448
6	5.699924	1.194258	0.378516
6	6.270352	0.260831	-0.489942
6	5.481446	-0.783052	-0.988224
6	4.139893	-0.889807	-0.626464
6	-2.015370	-2.689577	-1.854429
1	-1.612414	-2.163747	-2.724994
1	-1.254789	-3.306057	-1.377486
1	-3.185199	-0.175121	-2.628968
1	-4.153785	0.270635	-1.191900
1	-0.687358	-0.326791	-1.425494
1	-0.084764	-3.073437	0.950490
1	-4.511016	-1.245129	-2.061776
1	-2.867552	-3.308126	-2.151777
1	-1.925573	-3.292455	2.522265
1	1.414765	-1.573833	-0.570530
1	1.850019	0.720806	1.414592
1	-0.339457	-0.147851	1.530235
1	3.552221	-1.717169	-1.014837
1	5.917244	-1.521222	-1.657408
1	7.317126	0.339724	-0.771883
1	6.300903	2.007501	0.778057
1	3.920018	1.816046	1.417528
1	-0.867094	1.883104	-2.105039
1	-1.638802	4.211302	-1.757867
1	-2.902624	4.809225	0.302626
1	-3.369974	3.065061	2.016271
1	-2.573663	0.724485	1.675392

$E_{(MeCN)}$ = -1248.934068
NImag = 0

36. **2a**-$R^{‡}$ conformer 1 (-1248.701759)

6	0.419457	1.888904	-0.771200
6	1.223860	1.449707	0.294957
6	1.504714	2.344376	1.339206
6	0.989440	3.644170	1.326737
6	0.198413	4.071596	0.258313
6	-0.082201	3.190609	-0.791969
6	1.768589	0.042082	0.366918
16	2.882507	-0.214382	-1.140155
6	4.087946	1.146238	-0.997357
6	0.745907	-1.189778	0.433520
6	1.091002	-2.130586	1.555543
6	1.712663	-3.343326	1.313795
8	2.174153	-3.763549	0.192557
6	-0.687531	-0.738447	0.554270
6	-1.652690	-1.046254	-0.330732
6	-3.086158	-0.728942	-0.240065
6	-3.921482	-1.040707	-1.330268
6	-5.287514	-0.753541	-1.306502
6	-5.856846	-0.146304	-0.184603
6	-5.043136	0.164735	0.911703
6	-3.679889	-0.122944	0.885892
6	3.893514	-1.662720	-0.710115
1	4.529514	-1.419436	0.145454
1	3.207161	-2.516950	-0.459861
1	4.544173	1.140755	-0.004039
1	3.567423	2.089125	-1.172639
1	2.454890	-0.051279	1.213841
1	0.714622	-1.906559	2.552221
1	4.849754	0.990452	-1.765382
1	4.494544	-1.896658	-1.593186
1	1.828843	-4.006731	2.194268
1	-0.934203	-0.186583	1.461593
1	-1.365532	-1.603355	-1.224364
1	0.841399	-1.758254	-0.503044
1	-3.072595	0.115884	1.754466

1	-5.476202	0.628847	1.794789
1	-6.920471	0.076489	-0.159360
1	-5.906805	-1.008217	-2.163320
1	-3.488465	-1.519017	-2.206693
1	2.118315	2.016380	2.175568
1	1.208647	4.319075	2.150006
1	-0.201792	5.081904	0.244270
1	-0.705314	3.512701	-1.622000
1	0.170418	1.206717	-1.578806

$E_{(MeCN)}$ = -1248.930652
NImag = 1 (-16.8)

37. **2a**-R‡ conformer 2 (-1248.678792)

6	2.994418	-0.036509	1.220907
6	2.649278	0.145160	-0.129371
6	3.668608	0.218523	-1.088582
6	5.010273	0.126882	-0.712144
6	5.346408	-0.032958	0.635367
6	4.337771	-0.112492	1.599755
6	1.217809	0.244515	-0.564799
16	0.487996	1.831298	0.249243
6	1.812775	3.078948	0.093565
6	0.250403	-1.037615	-0.281194
6	0.827753	-2.099438	0.585255
6	1.729559	-2.991459	0.000511
8	2.186012	-2.905967	-1.176216
6	-1.130834	-0.677346	0.192912
6	-2.238620	-0.699834	-0.576946
6	-3.625751	-0.442701	-0.160616
6	-4.623388	-0.328679	-1.149063
6	-5.952879	-0.066260	-0.813806
6	-6.321488	0.085463	0.525280
6	-5.345741	-0.036212	1.522284
6	-4.018927	-0.298278	1.186269
6	-0.666527	2.479557	-1.007331
1	-0.154039	2.571155	-1.968658
1	-1.498412	1.778144	-1.075047
1	2.183479	3.116397	-0.933326
1	2.618981	2.792421	0.769169
1	1.170580	0.499992	-1.629735
1	0.484853	-2.229926	1.608985
1	1.392117	4.042766	0.394268
1	-1.021662	3.455085	-0.665417
1	2.071910	-3.832318	0.644377
1	-1.221380	-0.452228	1.257439
1	-2.116543	-0.944909	-1.634008
1	0.186349	-1.443303	-1.301089
1	-3.284875	-0.413549	1.978941
1	-5.623920	0.062471	2.568899
1	-7.356196	0.284396	0.791870
1	-6.700982	0.013669	-1.598793
1	-4.348149	-0.454238	-2.194603
1	3.408370	0.308614	-2.140596
1	5.787601	0.165832	-1.470384
1	6.389775	-0.106894	0.931618
1	4.593887	-0.254665	2.646481
1	2.216814	-0.127551	1.971921

$E_{(MeCN)}$ = -1248.915720
NImag = 1 (-25.8)

38. **2a**-*t*‡ (-1248.716781) [$PCM_{(MeCN)}$/B3LYP/6-31+G* geometry]

6	-1.636281	1.903960	0.199133
6	-2.279565	0.685475	-0.080888
6	-3.565323	0.715150	-0.644776
6	-4.184977	1.931424	-0.946621
6	-3.532933	3.138037	-0.673646
6	-2.259865	3.120383	-0.093966
6	-1.642191	-0.661722	0.194291
16	-1.116838	-0.641906	2.033382
6	-2.720795	-0.529780	2.891845
6	-0.445030	-1.112124	-0.706986
6	-0.937403	-1.196958	-2.132230
6	-1.091408	-2.393221	-2.800667
8	-0.889026	-3.593256	-2.367711
6	0.793110	-0.253932	-0.597862
6	1.989366	-0.705267	-0.172691
6	3.259981	0.039446	-0.116969
6	4.366781	-0.559603	0.517312
6	5.594524	0.101375	0.612501
6	5.746099	1.380986	0.068848
6	4.658206	1.987279	-0.574369
6	3.433002	1.326157	-0.668771
6	-0.685366	-2.379192	2.364312
1	-1.448958	-3.044509	1.951298
1	0.289074	-2.579480	1.916797
1	-3.399972	-1.305914	2.528797
1	-3.128894	0.463997	2.699016
1	-2.404657	-1.450369	0.150280
1	-1.162493	-0.269722	-2.657077
1	-2.526009	-0.650046	3.961138
1	-0.617906	-2.492877	3.450034
1	-1.435014	-2.292027	-3.853684
1	0.694810	0.770217	-0.958449
1	2.060665	-1.743160	0.164974
1	-0.194620	-2.137050	-0.406830

1	2.609731	1.813799	-1.188118
1	4.767622	2.980089	-1.010625
1	6.701684	1.899827	0.138585
1	6.432901	-0.385665	1.110360
1	4.258872	-1.558268	0.942371
1	-4.080021	-0.221985	-0.856898
1	-5.180390	1.933482	-1.390064
1	-4.016359	4.087055	-0.903710
1	-1.747283	4.054620	0.132832
1	-0.650765	1.917285	0.659750

$E_{(MeCN)}$ = -1248.928475
NImag = 0

39. **2a**-E‡ conformer (-1242.432530) [HF/6-31+G* geometry]

6	-4.138016	-0.929775	-0.929704
6	-3.309279	-0.446533	0.081534
6	-3.813878	0.540195	0.930557
6	-5.093167	1.040706	0.754728
6	-5.902207	0.561075	-0.267272
6	-5.419879	-0.430093	-1.107392
6	-1.941226	-0.999857	0.217280
6	-0.908252	-0.412347	0.804740
6	0.447371	-1.042470	0.948782
6	1.004844	-0.992487	2.352381
6	2.049300	-1.844469	2.659448
8	2.626152	-2.604737	1.853126
6	1.601875	-0.342090	0.261575
16	1.688462	-1.072665	-1.824895
6	3.347138	-0.522517	-2.279568
6	1.720581	1.142026	0.123429
6	2.831781	1.768989	0.682144
6	2.993332	3.142916	0.583436
6	2.051595	3.904180	-0.091727
6	0.947466	3.287344	-0.664640
6	0.780596	1.916180	-0.555502
6	1.992572	-2.835614	-1.528049
1	0.561332	-0.346986	3.087689
1	0.411322	-2.070732	0.609844
1	2.522017	-0.835443	0.501416
1	3.636276	-0.993012	-3.209954
1	4.055608	-0.777461	-1.502253
1	3.319434	0.549059	-2.413252
1	2.540041	-2.973722	-0.604667
1	1.033903	-3.328031	-1.456035
1	2.533729	-3.240824	-2.373171
1	-0.076102	1.450805	-1.006073
1	0.215940	3.871893	-1.193086
1	2.175928	4.969303	-0.172731
1	3.848992	3.613687	1.033088
1	3.557221	1.182095	1.215991
1	2.400264	-1.824384	3.694978
1	-1.025439	0.564424	1.243040
1	-1.800362	-1.974614	-0.223656
1	-3.215131	0.904864	1.745039
1	-5.463804	1.797459	1.423542
1	-6.897036	0.948005	-0.398306
1	-6.038713	-0.816852	-1.897798
1	-3.775300	-1.701128	-1.587412

$E_{(MeCN)}$ = -1248.923583
NImag = 1 (-370.5)

40. **2a**-PC (-1248.777873)

6	-4.504751	-2.140689	-0.408614
6	-3.679053	-1.040061	-0.110706
6	-4.287138	0.226162	0.006152
6	-5.662643	0.377482	-0.156208
6	-6.469884	-0.729658	-0.444764
6	-5.882990	-1.990732	-0.571864
6	-2.235994	-1.263859	0.059361
6	-1.312077	-0.373677	0.469597
6	0.120437	-0.697431	0.596153
6	0.891599	-0.214343	1.861961
6	1.815338	-1.167108	2.508173
8	2.573747	-1.915936	1.910430
6	1.207303	0.337784	0.482369
16	4.494613	-1.158538	-1.548261
6	5.555103	-1.016971	-0.066362
6	0.926945	1.772696	0.142166
6	1.117997	2.806320	1.069110
6	0.894049	4.139734	0.711529
6	0.477512	4.458100	-0.583076
6	0.288759	3.435023	-1.518113
6	0.511771	2.104937	-1.157649
6	3.945794	-2.891053	-1.350882
1	0.407607	-1.698281	0.279525
1	2.133541	-0.056047	0.060158
1	6.405868	-1.704227	-0.125146
1	4.978064	-1.217806	0.841202
1	5.934121	0.008745	-0.034906
1	3.423012	-3.021970	-0.398963
1	3.259888	-3.109786	-2.174682
1	4.794510	-3.580932	-1.409337
1	0.363405	1.312724	-1.887510
1	-0.033187	3.672652	-2.528992
1	0.303088	5.493921	-0.862870

1	1.048891	4.927676	1.444560
1	1.450871	2.568829	2.076677
1	1.783752	-1.186417	3.617964
1	-1.602496	0.644660	0.722459
1	-1.900200	-2.275704	-0.173267
1	-3.680234	1.102431	0.216195
1	-6.108021	1.364976	-0.063036
1	-7.542230	-0.607180	-0.572752
1	-6.496699	-2.858909	-0.799034
1	-4.056188	-3.126967	-0.508702
1	0.320409	0.415766	2.539191

$E_{(MeCN)}$ = -1248.984792
NImag = 0

41. **2b**-A-*c*‡ conformer 1 (-1248.695769)

6	4.310180	-1.445392	-0.518996
6	3.373297	-0.593493	0.097882
6	3.809036	0.691018	0.484450
6	5.123476	1.097311	0.265690
6	6.041817	0.235555	-0.346965
6	5.627578	-1.039704	-0.738765
6	2.001379	-1.076250	0.300968
6	0.993900	-0.450634	0.945566
6	-0.350904	-1.016126	1.121611
6	-1.080058	-0.677760	2.286112
6	-2.292468	-1.328431	2.594111
8	-2.870364	-2.167982	1.853810
6	-1.281017	-0.240994	-0.623200
16	-2.805420	-1.091218	-0.991772
6	-3.093159	-0.815899	-2.797269
6	-1.480821	1.201323	-0.404325
6	-2.489903	1.702207	0.447770
6	-2.591677	3.070973	0.706909
6	-1.685211	3.973236	0.143806
6	-0.669355	3.489694	-0.689072
6	-0.571325	2.125847	-0.963005
6	-2.370260	-2.856261	-1.045494
1	-1.442109	-3.002455	-1.604970
1	-2.287960	-3.163885	-0.001206
1	-3.990628	-1.364048	-3.100949
1	-2.224059	-1.146957	-3.372657
1	-0.535758	-0.485916	-1.383791
1	-0.749988	0.144371	2.916398
1	-3.249128	0.256393	-2.933236
1	-3.197036	-3.381064	-1.531105
1	-2.778496	-1.049439	3.550870
1	-0.458848	-2.040632	0.772147
1	1.154599	0.531458	1.388121

1	1.802284	-2.067503	-0.111619
1	3.997147	-2.441764	-0.824965
1	6.329382	-1.720168	-1.214840
1	7.066352	0.556821	-0.515762
1	5.434703	2.092787	0.573135
1	3.113929	1.379212	0.956809
1	0.219922	1.763593	-1.615979
1	0.043918	4.178523	-1.135885
1	-1.767818	5.037195	0.349717
1	-3.381388	3.430867	1.362260
1	-3.196408	1.018638	0.908675

$E_{(MeCN)}$ = -1248.913873
NImag = 1 (-274.2)

42. **2b**-A-*c*‡ conformer 2 (-1248.684194)

6	3.767858	0.924502	-0.807750
6	3.070361	-0.250033	-0.463471
6	3.755397	-1.220707	0.296580
6	5.072492	-1.015675	0.702939
6	5.746329	0.162878	0.359887
6	5.086871	1.131646	-0.400624
6	1.679676	-0.405270	-0.912769
6	0.806407	-1.371766	-0.559301
6	-0.571085	-1.480770	-1.070084
6	-1.160556	-2.777273	-1.134049
6	-2.418148	-2.969897	-1.749302
8	-3.152882	-2.055810	-2.201351
6	-1.806080	-0.301444	0.033154
16	-1.956651	-1.057040	1.624837
6	-0.589226	-0.464749	2.680145
6	-1.703435	1.166453	-0.115719
6	-0.649558	1.948796	0.406440
6	-0.583290	3.322917	0.164147
6	-1.546837	3.952052	-0.629405
6	-2.575775	3.186928	-1.188625
6	-2.654043	1.817961	-0.934748
6	-3.355086	-0.278467	2.533590
1	-3.236495	0.807671	2.540211
1	-4.269200	-0.556652	2.004741
1	-0.649428	-1.015787	3.622479
1	-0.668939	0.609137	2.858404
1	-2.649037	-0.716881	-0.530516
1	-0.683973	-3.618611	-0.634168
1	0.346578	-0.701125	2.171003
1	-3.379180	-0.678247	3.552095
1	-2.780352	-4.019075	-1.804162
1	-0.789755	-0.823838	-1.912344
1	1.117699	-2.157513	0.131667

1	1.332016	0.362228	-1.604510
1	3.262443	1.682551	-1.402468
1	5.599935	2.048218	-0.681303
1	6.775027	0.317442	0.674864
1	5.580986	-1.782917	1.281950
1	3.261573	-2.153420	0.555391
1	-3.452758	1.230277	-1.381140
1	-3.322590	3.657672	-1.823425
1	-1.487599	5.020034	-0.822195
1	0.238530	3.899702	0.582190
1	0.150362	1.479771	0.968455

$E_{(MeCN)}$ = -1248.905393
NImag = 1 (-292.3)

43. **2b**-A-$c^{‡}$ conformer 3 (-1248.680512)

6	-0.180188	2.261797	-0.741889
6	-1.141487	1.390441	-0.188621
6	-1.816023	1.805199	0.981146
6	-1.538155	3.043937	1.563551
6	-0.581143	3.895207	1.004147
6	0.100288	3.493140	-0.150326
6	-1.346220	0.050812	-0.784359
6	-0.574237	-1.383377	0.371066
6	-1.318088	-1.611954	1.566856
6	-2.273935	-2.650770	1.672649
8	-3.022306	-2.915940	2.629757
6	0.804753	-0.862794	0.498300
6	1.830229	-1.248710	-0.286398
6	3.234259	-0.821814	-0.205992
6	4.164741	-1.373281	-1.107781
6	5.510818	-1.004319	-1.080836
6	5.961866	-0.069900	-0.145675
6	5.050830	0.488632	0.759366
6	3.707546	0.120240	0.730233
16	-3.100025	-0.337999	-0.896803
6	-3.136982	-1.874444	-1.869148
6	-3.815373	0.827186	-2.116577
1	-2.512242	-1.772214	-2.760462
1	-2.776515	-2.678157	-1.225939
1	-4.877391	0.593484	-2.237639
1	-3.287717	0.752960	-3.070494
1	-0.893680	-0.060012	-1.774531
1	-1.159523	-0.970600	2.431973
1	-3.701117	1.829770	-1.699603
1	-4.176590	-2.068185	-2.143629
1	-2.322284	-3.321302	0.768623
1	-0.641077	-2.191217	-0.363193
1	0.963907	-0.148214	1.303711
1	1.623306	-1.978370	-1.072256
1	3.823412	-2.105403	-1.837203
1	6.206304	-1.449178	-1.788444
1	7.009174	0.219636	-0.118532
1	5.390826	1.215581	1.493074
1	3.020956	0.567777	1.443060
1	0.358449	1.959886	-1.637350
1	0.849722	4.142750	-0.595950
1	-0.368438	4.858293	1.460365
1	-2.068953	3.338847	2.465436
1	-2.542668	1.148001	1.451516

$E_{(MeCN)}$ = -1248.910041
NImag = 1 (-319.6)

44. **2b**-A-$t^{‡}$ (-1248.677512)

6	-4.238506	-0.125780	1.512101
6	-3.501955	-0.512095	0.374585
6	-4.201301	-0.644431	-0.843511
6	-5.569295	-0.387647	-0.917941
6	-6.282168	0.004562	0.221438
6	-5.608556	0.130777	1.439049
6	-2.057676	-0.750912	0.510626
6	-1.166985	-0.984766	-0.476921
6	0.264220	-1.256065	-0.256853
6	0.874061	-2.221019	-1.099610
6	1.925864	-3.074547	-0.650488
8	2.466083	-3.072282	0.469797
6	1.225274	0.481436	-0.605357
16	0.485476	2.015755	0.022484
6	1.526882	3.474212	-0.456936
6	2.606370	0.345172	-0.064946
6	2.874772	0.397445	1.317565
6	4.164690	0.198016	1.802971
6	5.216320	-0.078355	0.921829
6	4.963856	-0.143514	-0.449070
6	3.674432	0.077564	-0.939064
6	-0.914510	2.309907	-1.104146
1	-0.572578	2.259275	-2.141636
1	-1.667040	1.547464	-0.907911
1	1.031478	4.387688	-0.113524
1	1.669588	3.487470	-1.540464
1	1.202044	0.528963	-1.698140
1	0.498639	-2.365753	-2.112492
1	2.486442	3.352476	0.048544
1	-1.319287	3.300293	-0.882260
1	2.254956	-3.830299	-1.400850
1	0.551913	-1.335452	0.791486
1	-1.500512	-1.022272	-1.515388
1	-1.684113	-0.731388	1.535745
1	-3.723837	-0.029772	2.466070

1	-6.150059	0.425197	2.334763
1	-7.349726	0.199078	0.160531
1	-6.085429	-0.504070	-1.867964
1	-3.675902	-0.971184	-1.736886
1	3.486463	0.023603	-2.008493
1	5.770059	-0.370371	-1.142320
1	6.218365	-0.253432	1.304230
1	4.345819	0.228591	2.874398
1	2.061687	0.560313	2.022518

$E_{(MeCN)}$ = -1248.904698
NImag = 1 (-327.5)

45. **2b**-*c* (-1248.714410)

6	4.469398	-1.404180	-0.489353
6	3.463474	-0.549698	-0.001091
6	3.835621	0.757710	0.370233
6	5.157411	1.185016	0.260881
6	6.145880	0.320470	-0.225110
6	5.794545	-0.978110	-0.600241
6	2.084026	-1.058071	0.092859
6	1.009845	-0.428445	0.598125
6	-0.373318	-1.033033	0.676359
6	-0.908952	-1.011218	2.084486
6	-2.101784	-1.619104	2.362832
8	-2.880685	-2.146759	1.471271
6	-1.241375	-0.296706	-0.415670
16	-2.929571	-1.105489	-0.731837
6	-3.139636	-0.444359	-2.456457
6	-1.489377	1.176246	-0.192859
6	-2.292499	1.646239	0.860741
6	-2.462015	3.019522	1.058301
6	-1.833410	3.940471	0.216027
6	-1.032915	3.482286	-0.834668
6	-0.868849	2.110473	-1.038978
6	-2.560281	-2.822717	-1.224325
1	-1.639933	-2.855603	-1.814776
1	-2.477906	-3.388859	-0.298383
1	-4.074402	-0.854202	-2.849950
1	-2.305070	-0.717549	-3.110200
1	-0.728750	-0.433514	-1.375222
1	-0.303464	-0.578237	2.875224
1	-3.223353	0.642311	-2.390319
1	-3.403516	-3.171693	-1.826672
1	-2.442849	-1.651755	3.412655
1	-0.301204	-2.072921	0.316542
1	1.102370	0.576403	1.008789
1	1.949793	-2.074429	-0.282916
1	4.205614	-2.418931	-0.780901
1	6.551036	-1.661515	-0.978225
1	7.175901	0.657334	-0.308822
1	5.419191	2.198418	0.555630
1	3.086277	1.447403	0.748289
1	-0.239368	1.760704	-1.854754
1	-0.538490	4.189397	-1.495912
1	-1.967788	5.007413	0.375038
1	-3.086188	3.367906	1.877161
1	-2.774020	0.937055	1.524397

$E_{(MeCN)}$ = -1248.935164
NImag = 0

46. **2b**-$R^{‡}$ (-1248.688785)

6	4.788277	0.054130	-0.819462
6	3.717291	-0.260654	0.039437
6	4.015869	-0.499087	1.396665
6	5.325850	-0.430754	1.866625
6	6.378309	-0.117984	0.997383
6	6.101384	0.123439	-0.350353
6	2.354949	-0.301478	-0.514417
6	1.208276	-0.596877	0.125864
6	-0.150112	-0.670905	-0.524188
6	-0.640148	-2.083241	-0.607285
6	-1.330565	-2.457790	-1.751616
8	-1.731061	-1.664598	-2.668493
6	-1.130427	0.357941	0.217162
16	-1.427681	1.815855	-0.983239
6	-2.261237	3.071232	0.043109
6	-2.505353	-0.078011	0.653184
6	-3.428673	-0.620466	-0.257433
6	-4.707123	-0.971273	0.181065
6	-5.073871	-0.803966	1.521098
6	-4.154571	-0.278966	2.432582
6	-2.879036	0.090763	1.995598
6	0.213736	2.590776	-1.157833
1	0.651177	2.793977	-0.177817
1	0.848653	1.899101	-1.710972
1	-2.371444	3.979419	-0.556061
1	-1.683960	3.273905	0.948851
1	-0.614214	0.829896	1.063350
1	-0.354937	-2.806751	0.151579
1	-3.244510	2.676237	0.303131
1	0.083827	3.513859	-1.728765
1	-1.568111	-3.537600	-1.851298
1	-0.076081	-0.336962	-1.571810
1	1.232536	-0.857857	1.186149
1	2.297015	-0.088906	-1.584112
1	4.584459	0.237003	-1.872776
1	6.907782	0.362979	-1.039338
1	7.399012	-0.067211	1.367398

1	5.529097	-0.625008	2.917150
1	3.218077	-0.749131	2.090664
1	-2.163839	0.495198	2.710161
1	-4.426179	-0.154934	3.477818
1	-6.068643	-1.089195	1.854532
1	-5.413184	-1.396395	-0.527544
1	-3.132098	-0.789502	-1.293615

$E_{(MeCN)}$ = -1248.924140
NImag = 1 (-24.8)

47. **2b**-*t* (-1248.701264)

16	-1.266408	-1.486702	-1.541427
6	-2.521784	-2.485354	-0.687997
6	-2.182149	-0.831588	-2.973005
6	-0.965227	0.032211	-0.442401
6	-0.049013	-0.500687	0.782996
6	-0.576050	-0.291140	2.168262
6	-1.401739	-1.228491	2.752563
8	-1.925607	-2.249588	2.170630
1	-2.237026	-2.513232	0.391826
1	-2.493414	-3.480147	-1.140038
1	-3.503475	-2.023454	-0.811667
1	-2.487221	-1.682454	-3.587799
1	-3.052420	-0.262728	-2.637629
1	-1.505940	-0.191179	-3.544355
1	-0.312945	0.597575	-1.119047
1	0.052668	-1.587086	0.635575
1	-0.216918	0.557523	2.745050
6	-2.207196	0.842238	-0.197403
6	-3.234502	0.425499	0.669796
6	-4.362405	1.229279	0.852476
6	-4.478502	2.459186	0.197096
6	-3.457188	2.889168	-0.653300
6	-2.334136	2.081065	-0.849786
1	-3.149599	-0.514296	1.204922
1	-5.146644	0.897033	1.527802
1	-5.355773	3.081581	0.354914
1	-3.530396	3.847345	-1.161262
1	-1.537091	2.426293	-1.506356
1	-1.658295	-1.064433	3.817384
6	1.316180	0.120139	0.621953
6	2.419231	-0.546046	0.237198
1	1.371897	1.183722	0.860922
1	2.318519	-1.609490	0.012762
6	3.785102	-0.016631	0.089073
6	4.152330	1.298673	0.437799
6	5.460198	1.748150	0.266114
6	6.441981	0.896998	-0.255639
6	6.097964	-0.412291	-0.599809
6	4.786824	-0.860095	-0.427669
1	3.412300	1.973858	0.858410
1	5.718074	2.766518	0.547158
1	7.461770	1.250166	-0.385026
1	6.850156	-1.087822	-1.000104
1	4.529630	-1.883040	-0.695556

$E_{(MeCN)}$ = -1248.92987
NImag = 0

48. **2b**-$E^{‡}$ (-1248.696919)

16	-0.730667	-1.755154	0.886511
6	-1.703951	-1.188954	2.323106
6	-1.755826	-3.146241	0.310623
6	-1.035026	-0.227383	-0.436078
6	-0.086712	0.890658	0.105018
6	-0.562165	2.264230	-0.268058
6	-1.221083	3.002069	0.707178
8	-1.587620	2.561455	1.849128
1	-1.395778	-0.166421	2.561227
1	-1.483559	-1.859083	3.157688
1	-2.768387	-1.199401	2.081413
1	-1.825659	-3.882684	1.116262
1	-2.748165	-2.788986	0.023953
1	-1.252762	-3.595743	-0.548811
1	-0.583953	-0.698165	-1.317775
1	-0.100140	0.872979	1.203503
1	-0.286396	2.699241	-1.224837
6	-2.505216	-0.061934	-0.662180
6	-3.349210	0.654203	0.208464
6	-4.718893	0.721990	-0.047804
6	-5.273930	0.083475	-1.163549
6	-4.444816	-0.621046	-2.039010
6	-3.072687	-0.693307	-1.786068
1	-2.922839	1.202736	1.048896
1	-5.354306	1.295740	0.622116
1	-6.342174	0.146901	-1.355299
1	-4.859259	-1.105276	-2.919638
1	-2.429479	-1.224229	-2.486114
1	-1.453570	4.056484	0.455825
6	1.317448	0.632554	-0.381652
6	2.369955	0.349032	0.406519
1	1.456369	0.729872	-1.460422
1	2.193883	0.255511	1.479555
6	3.769092	0.150687	-0.005490
6	4.238336	0.411958	-1.308676
6	5.571617	0.191347	-1.649218
6	6.478067	-0.290902	-0.697324
6	6.033468	-0.544298	0.602545
6	4.697119	-0.323573	0.941192

1	3.558901	0.806534	-2.059031
1	5.909146	0.405628	-2.660548
1	7.518215	-0.457442	-0.965348
1	6.727143	-0.910711	1.355499
1	4.360884	-0.520046	1.957456

$E_{(MeCN)}$ = -1248.927110
NImag = 1 (-83.9)

50. **2b**-PC (-1248.774421)

16	0.875941	3.159984	0.505640
6	1.099646	3.348934	-1.297558
6	0.918036	4.913576	1.014743
6	-1.687514	-0.145069	0.514674
6	-0.646704	-1.228380	0.562584
6	-1.415507	-0.904746	1.845003
6	-2.375377	-1.887661	2.393721
8	-2.835043	-2.840609	1.787621
1	1.090209	2.345447	-1.731581
1	2.059336	3.822854	-1.527269
1	0.283790	3.931854	-1.736968
1	1.877626	5.375087	0.760057
1	0.102672	5.478778	0.551649
1	0.792357	4.939109	2.100773
1	-1.279223	0.863397	0.566538
1	-0.935327	-2.184043	0.129411
1	-0.907178	-0.307768	2.599887
6	-2.967116	-0.200719	-0.255301
6	-3.474118	-1.363458	-0.857203
6	-4.667591	-1.327060	-1.582435
6	-5.376709	-0.131664	-1.724246
6	-4.881065	1.033891	-1.133134
6	-3.689153	0.996361	-0.408168
1	-2.949013	-2.305751	-0.750399
1	-5.043310	-2.240488	-2.036665
1	-6.304122	-0.107830	-2.290876
1	-5.419317	1.972812	-1.238131
1	-3.306656	1.908858	0.044841
1	-2.676181	-1.706237	3.447687
6	0.789613	-0.891798	0.466591
6	1.706209	-1.683646	-0.120238
1	1.083870	0.062096	0.904139
1	1.365969	-2.631129	-0.540695
6	3.147130	-1.426357	-0.267510
6	3.775148	-0.243934	0.174555
6	5.146392	-0.058389	0.009752
6	5.930079	-1.044866	-0.601475
6	5.323554	-2.221280	-1.047387
6	3.949710	-2.406452	-0.881562
1	3.190905	0.540753	0.647603
1	5.607492	0.862121	0.359767
1	6.999309	-0.895575	-0.727660
1	5.918319	-2.996468	-1.524294
1	3.485780	-3.326450	-1.231468

$E_{(MeCN)}$ = -1248.978790
NImag = 0

<u>1,6-Addition (Pathway 3)</u>

51. **3a**-A-$c^{\ddagger}$ conformer 1 (-1248.684690)

6	2.595135	-1.409117	0.460947
6	1.250646	-1.425103	0.033245
6	0.941168	-2.156164	-1.136150
6	1.930637	-2.855603	-1.828854
6	3.257484	-2.831731	-1.388146
6	3.583040	-2.097425	-0.242488
6	0.241837	-0.617859	0.748098
16	-1.286592	-1.528681	1.019983
6	-0.851211	-3.016008	2.002565
6	-2.135430	-0.552831	2.298000
6	-0.258887	1.005876	-0.396780
6	-1.546546	1.573062	-0.158776
6	-2.714174	1.052808	-0.730214
6	-4.025770	1.465892	-0.533581
6	-5.134609	0.794638	-1.153886
8	-5.082977	-0.219567	-1.868134
6	0.957831	1.834348	-0.149822
6	1.100062	2.619679	1.008747
6	2.237045	3.402116	1.212191
6	3.262699	3.416214	0.260257
6	3.138138	2.637694	-0.892638
6	2.000321	1.850936	-1.090650
1	-6.130146	1.247317	-0.943413
1	-4.248499	2.328589	0.094767
1	-2.601658	0.205274	-1.411970
1	-1.626015	2.423425	0.518644
1	0.588040	-0.216410	1.703091
1	-1.777065	-3.545772	2.246297
1	-0.216264	-3.642865	1.373840
1	-0.315639	-2.722361	2.908508
1	-3.040307	-1.096604	2.578811
1	-1.474981	-0.415562	3.158372
1	-2.399829	0.399614	1.838407
1	-0.189726	0.422711	-1.315974
1	1.912928	1.248652	-1.991592
1	3.927138	2.639836	-1.640702
1	4.146929	4.028899	0.416485
1	2.322231	4.004829	2.113390
1	0.310753	2.622638	1.756945
1	2.863125	-0.841265	1.348872
1	4.611373	-2.063600	0.109058

1	4.026770	-3.373677	-1.931384
1	1.662847	-3.413411	-2.722849
1	-0.079221	-2.173364	-1.514655

$E_{(MeCN)}$ = -1248.909936
NImag = 1 (-290.6)

52. **3a**-A-*c*‡ conformer 2 (-1248.682799)

6	-2.422113	-1.485279	-1.109936
6	-1.371450	-1.825478	-0.240579
6	-1.654328	-2.697193	0.827621
6	-2.936087	-3.216359	1.010453
6	-3.969526	-2.874977	0.130707
6	-3.705690	-2.007314	-0.931675
6	-0.012290	-1.264137	-0.471127
6	-0.196136	0.461855	0.724026
16	1.375512	0.723883	1.567806
6	1.082311	2.069774	2.784387
6	-0.849610	1.603012	0.049197
6	-2.094092	2.084994	0.511729
6	-2.775794	3.098895	-0.161390
6	-2.230018	3.670651	-1.315556
6	-1.005731	3.198934	-1.798818
6	-0.330806	2.172431	-1.135580
6	2.539176	1.607173	0.475585
6	1.156055	-2.020928	-0.183031
6	2.390750	-1.621550	-0.696637
6	3.673638	-2.091977	-0.446388
6	4.812133	-1.366203	-0.926529
8	4.787600	-0.250684	-1.485210
1	5.798164	-1.845695	-0.746943
1	3.846104	-2.984279	0.153279
1	2.360578	-0.781283	-1.395279
1	1.110722	-2.839070	0.532968
1	-0.807840	0.033040	1.521852
1	3.388580	1.876266	1.108682
1	2.899004	0.935232	-0.306910
1	2.068491	2.501892	0.065032
1	2.031866	2.308944	3.272488
1	0.670050	2.947588	2.281006
1	0.373683	1.691597	3.524382
1	0.045453	-0.662597	-1.377328
1	-2.226647	-0.811387	-1.940706
1	-4.498157	-1.735556	-1.624739
1	-4.966970	-3.283414	0.271786
1	-3.128718	-3.892590	1.840033
1	-0.864695	-2.977240	1.519965
1	-2.530762	1.647978	1.407250
1	-3.733539	3.446106	0.218765
1	-2.757463	4.464096	-1.838169
1	-0.580781	3.617874	-2.707706
1	0.591539	1.787889	-1.561690

$E_{(MeCN)}$ = -1248.904645
NImag = 1 (-278.0)

53. **3a**-A-*t*‡ (-1248.682050)

6	-0.667627	2.287694	-0.769495
6	0.311137	1.587813	-0.036241
6	1.666670	1.895076	-0.273872
6	2.026130	2.882224	-1.191339
6	1.043623	3.569001	-1.914053
6	-0.302186	3.260768	-1.703629
6	-0.135245	0.492794	0.868136
16	0.865141	0.460647	2.380636
6	0.409571	1.905849	3.449576
6	0.052020	-0.851580	3.351734
6	-0.356589	-1.191609	-0.072010
6	-1.397618	-0.965084	-1.028607
6	-2.744265	-1.010206	-0.652129
6	-3.873279	-0.738952	-1.410868
6	-5.194225	-0.819159	-0.850076
8	-5.486666	-1.098078	0.324337
6	1.000025	-1.630571	-0.518415
6	1.611326	-1.125909	-1.679975
6	2.875704	-1.566979	-2.074083
6	3.562812	-2.522145	-1.318104
6	2.968255	-3.038078	-0.164071
6	1.703487	-2.592466	0.227997
1	-6.018608	-0.595027	-1.563916
1	-3.786596	-0.458017	-2.459956
1	-2.957757	-1.300122	0.381244
1	-1.134865	-0.661793	-2.039534
1	-1.173656	0.618694	1.185442
1	0.924387	1.812094	4.410802
1	0.750110	2.801101	2.926121
1	-0.674373	1.934575	3.586351
1	0.456385	-0.814452	4.365971
1	-1.030876	-0.700905	3.363112
1	0.296537	-1.811471	2.897347
1	-0.701265	-1.770418	0.786552
1	1.237397	-3.029395	1.109932
1	3.481374	-3.794840	0.424533
1	4.544994	-2.867200	-1.630872
1	3.324807	-1.164522	-2.978876
1	1.094373	-0.386725	-2.283374
1	-1.717841	2.060372	-0.609601
1	-1.075981	3.782678	-2.260990
1	1.326270	4.334035	-2.632422
1	3.077964	3.105386	-1.352275

1	2.449934	1.349354	0.246670

$E_{(MeCN)}$ = -1248.909122
NImag = 1 (-341.5)

54. **3a**-*c* (-1248.703223)

6	0.361107	0.511450	0.111064
6	1.751372	0.315391	-0.445067
6	2.894820	0.213828	0.351050
6	4.222698	0.199706	-0.060081
6	5.301631	-0.046072	0.855947
8	5.207574	-0.309686	2.064646
6	-0.522093	-0.596348	-0.517735
6	-1.849350	-0.917512	0.109440
6	-1.972094	-1.129342	1.493451
6	-3.212557	-1.422212	2.060908
6	-4.353700	-1.501109	1.255457
6	-4.246171	-1.287062	-0.120931
6	-3.001708	-1.001930	-0.687356
16	0.753268	-2.042650	-0.479277
6	-0.435014	-3.469639	-0.770096
6	1.623491	-2.225952	-2.083404
1	2.611067	-1.782657	-1.956789
1	-1.003481	-3.347184	-1.697110
1	-1.116358	-3.528582	0.078996
1	-0.652743	-0.405521	-1.588944
1	0.171746	-4.377963	-0.814300
1	1.696772	-3.290316	-2.326195
1	-1.094242	-1.070900	2.132147
1	-3.289648	-1.584196	3.132776
1	-5.320133	-1.723826	1.699761
1	-5.128985	-1.338287	-0.752787
1	-2.926159	-0.827418	-1.758678
1	1.880045	0.576785	-1.498617
1	2.745738	0.058903	1.423115
1	4.484329	0.405307	-1.098618
1	6.317489	0.016375	0.402147
1	0.403391	0.329353	1.192028
6	-0.254953	1.891659	-0.100272
6	-0.441814	2.423297	-1.386530
6	-0.984756	3.696508	-1.566905
6	-1.351067	4.469005	-0.459903
6	-1.168163	3.953805	0.824985
6	-0.628467	2.676068	0.999475
1	-0.143699	1.848674	-2.261460
1	-1.114911	4.089242	-2.572545
1	-1.769204	5.462554	-0.599109
1	-1.443484	4.544945	1.694966
1	-0.486476	2.287319	2.005617

1	1.066793	-1.703949	-2.866115

$E_{(MeCN)}$ = -1248.931268
NImag = 0

55. **3a**-$R^{‡}$ (-1248.684548)

6	1.651901	1.961532	0.855968
6	0.841632	1.705459	-0.262238
6	1.215909	2.269104	-1.490649
6	2.361906	3.062383	-1.605368
6	3.159665	3.304813	-0.485316
6	2.796967	2.751153	0.747427
6	-0.438563	0.891112	-0.156996
6	-1.410581	1.403532	0.874907
6	-2.756894	1.256042	0.651695
6	-3.906969	1.398394	1.454514
6	-5.153981	0.947670	0.951431
8	-5.363793	0.371960	-0.149673
6	-0.190854	-0.680656	0.117783
16	-0.904425	-1.713051	-1.358746
6	-2.727308	-1.535495	-1.266960
6	1.195564	-1.214511	0.374123
6	2.222031	-1.134885	-0.583365
6	3.491938	-1.639032	-0.303947
6	3.763478	-2.215331	0.942279
6	2.754527	-2.291713	1.904675
6	1.475888	-1.805480	1.616628
6	-0.735799	-3.422283	-0.747925
1	-6.024025	1.107995	1.626035
1	-3.861145	1.794658	2.467370
1	-3.027096	0.936458	-0.356109
1	-1.009815	1.723015	1.835809
1	-0.860460	-0.967648	0.932269
1	-1.220163	-4.083138	-1.471094
1	0.327547	-3.655180	-0.682440
1	-1.209468	-3.516734	0.232667
1	-3.145798	-2.368505	-1.838188
1	-3.075279	-1.548215	-0.232643
1	-3.021527	-0.593469	-1.727046
1	-0.925615	0.954815	-1.140670
1	0.592503	2.101885	-2.367503
1	2.623814	3.495598	-2.567764
1	4.049543	3.923584	-0.568127
1	3.406026	2.938536	1.628520
1	1.382675	1.546063	1.823417
1	0.692898	-1.869148	2.369107
1	2.957459	-2.732070	2.877309
1	4.757053	-2.597385	1.161011

1	4.274902	-1.568490	-1.054171
1	2.034376	-0.660330	-1.542427

$E_{(MeCN)}$ = -1248.919513
NImag = 1 (-43.5)

56. **3a**-*t* conformer 1 (-1248.719348) [$PCM_{(MeCN)}$/B3LYP/6-31+G* geometry]

6	-1.565727	-1.154510	-1.301114
6	-0.732111	-1.559882	-0.242825
6	-0.384195	-2.920470	-0.149713
6	-0.844875	-3.846896	-1.088850
6	-1.669415	-3.428955	-2.137762
6	-2.027773	-2.080628	-2.239599
6	-0.183971	-0.619339	0.800432
16	-1.519375	-0.110771	2.112993
6	-1.956379	-1.716216	2.851007
6	0.653249	0.648177	0.403517
6	1.823194	0.171162	-0.425506
6	3.094820	0.113175	0.058325
6	4.272337	-0.327845	-0.632808
6	5.545448	-0.361933	-0.067261
8	5.906982	-0.030140	1.120199
6	-0.119966	1.827126	-0.194421
6	-0.346664	1.973543	-1.573765
6	-1.044328	3.077066	-2.074734
6	-1.520992	4.067173	-1.208041
6	-1.279558	3.950375	0.163891
6	-0.581122	2.843549	0.660946
6	-3.065168	0.276394	1.232980
1	6.344478	-0.730851	-0.747054
1	4.179973	-0.664401	-1.667474
1	3.254612	0.443860	1.089872
1	1.616946	-0.161817	-1.443709
1	0.470474	-1.189387	1.473236
1	-3.813081	0.481987	2.004598
1	-2.895341	1.174048	0.637342
1	-3.375381	-0.562721	0.607729
1	-2.787339	-1.541420	3.540075
1	-2.238700	-2.428678	2.072499
1	-1.084697	-2.070336	3.406735
1	1.058029	1.003321	1.362168
1	-0.376595	2.780643	1.731193
1	-1.623389	4.724196	0.850386
1	-2.061399	4.927997	-1.600672
1	-1.208747	3.165820	-3.148329
1	0.032664	1.231214	-2.271952
1	0.269332	-3.254921	0.657224
1	-0.555613	-4.893831	-0.999821
1	-2.030521	-4.148682	-2.871885
1	-2.670012	-1.744232	-3.052723
1	-1.852370	-0.114757	-1.407116

$E_{(MeCN)}$ = -1248.931645
NImag = 0

57. **3a**-*t* conformer 1 (-1242.408879) [HF/6-31+G* geometry]

6	0.960275	1.790848	-1.079086
6	-0.170049	1.506136	-0.315595
6	-1.306405	2.293623	-0.492455
6	-1.313303	3.342069	-1.399836
6	-0.178815	3.622515	-2.144900
6	0.956738	2.842372	-1.982954
6	-0.252609	0.369877	0.677131
16	0.839504	0.681216	2.243073
6	0.101643	2.164343	2.959517
6	-0.153683	-1.128177	0.230577
6	-1.299355	-1.337182	-0.725257
6	-2.556246	-1.548168	-0.245906
6	-3.792473	-1.637624	-0.910091
6	-4.983586	-1.785456	-0.169057
8	-5.112724	-1.827260	1.052303
6	1.218696	-1.595854	-0.236169
6	1.661497	-1.452372	-1.550745
6	2.915093	-1.902054	-1.935240
6	3.756504	-2.516849	-1.017019
6	3.323517	-2.688373	0.287293
6	2.066301	-2.234139	0.667455
6	2.475564	1.288134	1.783126
1	-5.892656	-1.857974	-0.781535
1	-3.852138	-1.587648	-1.984768
1	-2.652483	-1.657653	0.827013
1	-1.125019	-1.185129	-1.775787
1	-1.206710	0.433539	1.178707
1	3.016198	1.463210	2.703976
1	2.971950	0.515740	1.215865
1	2.397623	2.198847	1.210086
1	0.687231	2.450199	3.822872
1	0.078107	2.962885	2.232298
1	-0.901227	1.914241	3.275931
1	-0.369076	-1.681788	1.139124
1	1.732514	-2.409905	1.676430
1	3.949267	-3.190295	1.004267
1	4.723958	-2.874634	-1.321240
1	3.229380	-1.785695	-2.957521
1	1.022209	-1.000864	-2.285067
1	-2.204710	2.064398	0.052369
1	-2.207006	3.924597	-1.531477
1	-0.181923	4.432163	-2.852346

1	1.837113	3.042613	-2.567229
1	1.841298	1.185763	-0.994306

$E_{(MeCN)}$ = -1248.923132
NImag = 0

58. **3a**-*t* conformer 2 (-1242.414005) [HF/6-31+G* geometry]

6	-0.247092	-1.087635	-0.015429
6	-1.192826	-1.131520	-1.198085
6	-2.530966	-1.105712	-0.969781
6	-3.646550	-1.041794	-1.827530
6	-4.933126	-0.916033	-1.268642
8	-5.230987	-0.824185	-0.076463
6	-0.327259	0.376231	0.549236
6	0.376439	1.493357	-0.191217
6	1.747697	1.719314	-0.096589
6	2.337448	2.763553	-0.792184
6	1.566887	3.583898	-1.603846
6	0.203527	3.357560	-1.713476
6	-0.390228	2.322272	-1.005550
16	0.198600	0.464052	2.370131
6	-0.370383	2.108106	2.859781
6	-1.034791	-0.566253	3.201339
1	-1.402756	2.245767	2.569607
1	0.256673	2.838073	2.371952
1	-1.376548	0.612323	0.624360
1	-0.263955	2.190970	3.932869
1	2.366791	1.076954	0.503750
1	3.397102	2.926033	-0.709138
1	2.026567	4.389144	-2.148379
1	-0.400208	3.981676	-2.347164
1	-1.445688	2.144028	-1.105498
1	-0.782512	-1.110667	-2.190880
1	-2.834616	-1.117443	0.069988
1	-3.538946	-1.077270	-2.898514
1	-5.749856	-0.887072	-2.001374
1	-0.660230	-1.721508	0.762062
6	1.165355	-1.589297	-0.273131
6	1.863838	-1.284529	-1.440628
6	3.146178	-1.765327	-1.649891
6	3.763747	-2.564730	-0.697017
6	3.080986	-2.883940	0.464324
6	1.794326	-2.400665	0.666755
1	1.406919	-0.671509	-2.194000
1	3.661716	-1.520479	-2.561734
1	4.756842	-2.941692	-0.865249
1	3.536981	-3.517022	1.204947
1	1.269186	-2.688649	1.562418
1	-0.999272	-0.329392	4.256105
1	-0.772254	-1.602703	3.060821
1	-2.020887	-0.372032	2.802011

$E_{(MeCN)}$ = -1248.919653
NImag = 0

59. **3a**-$E^{‡}$ conformer 1 (-1242.408336) [HF/6-31+G* geometry]

6	1.049381	1.614838	-1.187805
6	-0.093804	1.479809	-0.401887
6	-1.127483	2.401298	-0.564344
6	-1.025161	3.430751	-1.487082
6	0.118686	3.557267	-2.259929
6	1.154293	2.646228	-2.107786
6	-0.284702	0.384539	0.608395
16	0.906409	0.767532	2.260453
6	0.166062	2.275695	2.921179
6	-0.228320	-1.119859	0.263633
6	-1.392642	-1.254763	-0.681017
6	-2.659915	-1.425310	-0.196089
6	-3.891173	-1.441201	-0.861881
6	-5.095266	-1.577631	-0.130339
8	-5.229379	-1.664996	1.084624
6	1.114618	-1.681580	-0.185264
6	1.513280	-1.719674	-1.520117
6	2.739586	-2.254888	-1.883905
6	3.594950	-2.775892	-0.922435
6	3.203867	-2.767481	0.406456
6	1.974605	-2.228673	0.765195
6	2.532776	1.368236	1.758999
1	-6.002587	-1.593128	-0.748921
1	-3.945765	-1.349381	-1.934036
1	-2.755524	-1.564305	0.872949
1	-1.226521	-1.070834	-1.727382
1	-1.203119	0.541577	1.147843
1	3.078546	1.630599	2.655906
1	3.042425	0.562948	1.251591
1	2.439094	2.225506	1.109696
1	0.751357	2.607943	3.768081
1	0.130255	3.044403	2.162303
1	-0.833677	2.035224	3.255325
1	-0.479622	-1.625025	1.189857
1	1.671744	-2.266152	1.798138
1	3.840222	-3.195298	1.161161
1	4.540637	-3.200263	-1.209010
1	3.020550	-2.277826	-2.922089
1	0.862082	-1.343905	-2.285583
1	-2.033599	2.291574	0.004447
1	-1.841618	4.119155	-1.609198
1	0.199898	4.351743	-2.979827

1	2.040881	2.731676	-2.710313
1	1.855002	0.912988	-1.099045

$E_{(MeCN)}$ = -1248.922948
NImag = 1 (-254.0)

60. **3a**-$E^{‡}$ conformer 2 (-1242.411372) [HF/6-31+G* geometry]

6	1.760611	-1.458880	-1.545359
6	1.186331	-1.614764	-0.285647
6	1.919936	-2.293133	0.683542
6	3.190515	-2.786612	0.419280
6	3.752168	-2.612615	-0.834674
6	3.028579	-1.949405	-1.815988
6	-0.204582	-1.102018	0.053054
6	-1.234080	-1.103775	-1.050578
6	-2.564553	-1.216636	-0.745824
6	-3.698823	-1.133409	-1.556407
6	-4.989544	-1.222538	-0.976156
8	-5.267290	-1.338981	0.210904
6	-0.317620	0.364295	0.486009
16	0.581900	0.663970	2.394446
6	-0.010495	2.317767	2.818679
6	-0.477785	-0.344175	3.457683
1	-5.817382	-1.167002	-1.694574
1	-3.617736	-1.005804	-2.622916
1	-2.807103	-1.389711	0.294899
1	-0.912168	-0.896076	-2.053921
1	-1.318328	0.556254	0.827041
1	0.196437	2.504672	3.863969
1	0.527659	3.029386	2.210807
1	-1.072262	2.401692	2.629126
1	-0.313374	-0.055593	4.487195
1	-1.519614	-0.211972	3.197286
1	-0.199297	-1.379746	3.334053
1	-0.578050	-1.701563	0.875419
1	1.490976	-2.465532	1.656260
1	3.729298	-3.314216	1.186384
1	4.732743	-2.998291	-1.049779
1	3.447728	-1.820124	-2.798192
1	1.221258	-0.957544	-2.325460
6	0.212569	1.500490	-0.341569
6	-0.702363	2.382261	-0.912814
6	-0.265399	3.453587	-1.676643
6	1.092720	3.663674	-1.864758
6	2.010849	2.795344	-1.291778
6	1.574573	1.716435	-0.537993
1	-1.756506	2.212216	-0.785984
1	-0.983748	4.116249	-2.124303
1	1.433449	4.496003	-2.454185
1	3.064927	2.951503	-1.435231
1	2.297373	1.048178	-0.108624

$E_{(MeCN)}$ = -1248.919954
NImag = 1 (-352.7)

61. **3a**-PC (-1248.774211)

6	0.297336	0.757221	0.015247
6	0.277172	-0.753128	-0.097682
16	-3.625574	0.395507	-1.749540
6	-5.096247	-0.291833	-0.910162
6	-3.939583	-0.172573	-3.457055
6	-0.093128	-0.111211	1.231222
6	-1.482049	-0.104147	1.689107
6	-1.887842	-0.102875	2.978247
6	-3.309384	-0.084155	3.347328
8	-4.249404	-0.071188	2.561478
1	-3.513107	-0.082128	4.438816
1	-1.167511	-0.112316	3.795422
1	-2.249473	-0.092856	0.914722
1	0.664761	-0.158912	2.010656
1	-0.580883	-1.117090	-0.664601
1	-4.872674	0.248837	-3.845337
1	-3.110378	0.179433	-4.077462
1	-3.980938	-1.265638	-3.509242
1	-6.013038	0.172197	-1.288223
1	-5.148319	-1.377296	-1.045806
1	-4.993321	-0.075485	0.156658
1	-0.551825	1.232605	-0.470868
6	1.513051	1.623368	0.029720
6	1.461649	2.846518	-0.660990
6	2.557271	3.711988	-0.683828
6	3.733434	3.371582	-0.011298
6	3.799017	2.158973	0.680974
6	2.702905	1.294311	0.701814
1	0.548510	3.123475	-1.183655
1	2.488432	4.652707	-1.224593
1	4.588365	4.042687	-0.024935
1	4.708796	1.880623	1.207210
1	2.785458	0.355620	1.240937
6	1.498664	-1.611332	-0.248117
6	1.845603	-2.560823	0.723584
6	2.951746	-3.396874	0.544740
6	3.726584	-3.296334	-0.613704
6	3.386734	-2.356110	-1.591507
6	2.282783	-1.520794	-1.408505
1	1.241195	-2.650358	1.623282
1	3.204754	-4.127710	1.309029

1	4.587728	-3.944708	-0.754174
1	3.985233	-2.268537	-2.494944
1	2.028370	-0.784379	-2.166880

$E_{(MeCN)}$ = -1248.978587
NImag = 0

62. **3b**-A-*c*‡ (-1248.682677)

6	-1.127910	-2.402328	-1.297825
6	-1.166227	-1.476035	-0.234979
6	-2.428863	-1.120994	0.286328
6	-3.597375	-1.684557	-0.224558
6	-3.543379	-2.600474	-1.281437
6	-2.301846	-2.949494	-1.819510
6	0.105713	-0.860923	0.222048
16	0.199041	-0.810019	2.011073
6	1.873240	-0.175173	2.373140
6	0.440141	-2.548208	2.578266
6	0.479992	0.858954	-0.693037
6	1.808852	1.334518	-0.453211
6	2.942014	0.653599	-0.901032
6	4.276134	0.923272	-0.618575
6	5.339149	0.080518	-1.092185
8	5.219507	-0.970994	-1.741834
6	-0.671958	1.764825	-0.403874
6	-0.748908	2.521305	0.779141
6	-1.828275	3.371885	1.023829
6	-2.860232	3.486834	0.086572
6	-2.799798	2.741161	-1.093263
6	-1.721005	1.885843	-1.330005
1	2.623398	-0.697622	1.775370
1	1.897830	0.884703	2.126792
1	1.303220	-2.984441	2.068839
1	-0.469923	-3.095793	2.326399
1	0.985831	-1.401528	-0.134343
1	0.354427	0.332256	-1.641989
1	0.587911	-2.540835	3.662543
1	2.037907	-0.326782	3.442906
1	-2.500384	-0.385323	1.083472
1	-4.557066	-1.395789	0.196913
1	-4.456858	-3.033132	-1.680344
1	-2.242364	-3.658134	-2.641867
1	-0.167129	-2.694700	-1.716417
1	1.938884	2.206806	0.187331
1	2.780483	-0.225684	-1.531502
1	4.552797	1.798222	-0.029908
1	6.362953	0.425854	-0.822370
1	-1.684793	1.309298	-2.251110
1	-3.593738	2.822568	-1.831563

1	-3.698991	4.152426	0.273678
1	-1.861404	3.949521	1.944579
1	0.049538	2.459208	1.515098

$E_{(MeCN)}$ = -1248.908011
NImag = 1 (-290.7)

63. **3b**-A-*t*‡ (-1248.678914)

6	-2.619082	-1.889963	-0.640183
6	-1.891881	-1.238281	0.372245
6	-2.596924	-0.810715	1.512453
6	-3.973780	-1.016711	1.637861
6	-4.682931	-1.655840	0.616856
6	-3.995656	-2.093853	-0.521138
6	-0.419184	-0.985897	0.286371
6	0.410933	-1.866117	-0.470917
6	1.763707	-2.089019	-0.177256
6	2.647512	-2.903857	-0.868608
6	4.016258	-3.075126	-0.465806
8	4.585570	-2.533403	0.494183
6	-0.196546	0.789172	-0.491725
6	1.124888	1.311682	-0.027083
6	1.305179	1.804959	1.281568
6	2.561896	2.216201	1.724604
6	3.673394	2.121467	0.880002
6	3.513319	1.615891	-0.410938
6	2.250618	1.224660	-0.863600
16	-1.443760	2.111789	-0.215042
6	-0.976643	3.625978	-1.180570
6	-2.871857	1.593886	-1.220639
1	-2.545724	1.352544	-2.235904
1	-3.328002	0.723660	-0.751451
1	-0.852548	3.367488	-2.235193
1	-0.033440	3.984310	-0.765175
1	-0.209586	0.566967	-1.562770
1	-0.003751	-0.726775	1.260998
1	-1.758508	4.380959	-1.051364
1	-3.580248	2.425973	-1.234267
1	0.460129	1.852642	1.966117
1	2.678001	2.589897	2.738845
1	4.656597	2.418767	1.233739
1	4.373654	1.509796	-1.065897
1	2.140379	0.820464	-1.866246
1	-0.006529	-2.358734	-1.348448
1	2.177582	-1.589195	0.700670
1	2.317918	-3.448069	-1.754014
1	4.603798	-3.769916	-1.109384
1	-2.053015	-0.323814	2.319692
1	-4.488821	-0.686964	2.537013

1	-5.752474	-1.824467	0.711784
1	-4.532261	-2.606652	-1.315949
1	-2.106866	-2.251372	-1.526576

$E_{(MeCN)}$ = -1248.908994
NImag = 1 (-357.2)

64. **3b**-*c* conformer 1 (-1248.699189)

6	2.327312	-2.061776	-1.372629
1	2.009555	-1.607231	-2.314391
1	3.122447	-1.476394	-0.912136
16	0.922737	-2.126862	-0.200797
6	0.072455	-3.609075	-0.989928
1	-0.057684	-3.476794	-2.068256
1	-0.896460	-3.732108	-0.503086
6	-0.345017	-0.821078	-0.744601
1	-0.537384	-0.996213	-1.809187
6	0.455159	0.509457	-0.519065
6	-0.488142	1.715457	-0.453426
1	1.045078	0.642337	-1.436968
6	1.451844	0.300151	0.595882
6	-1.627946	-1.059398	0.019194
1	0.698495	-4.481743	-0.787941
1	2.651411	-3.090601	-1.550344
6	-1.684156	-1.057129	1.423564
6	-2.892686	-1.274707	2.086548
6	-4.067593	-1.492093	1.360579
6	-4.025539	-1.494369	-0.035214
6	-2.813420	-1.285578	-0.697415
1	-0.783661	-0.884774	2.004193
1	-2.916286	-1.268805	3.173058
1	-5.008011	-1.656047	1.879925
1	-4.933111	-1.657645	-0.610344
1	-2.791605	-1.283930	-1.785048
1	1.071612	0.138334	1.604514
6	2.799073	0.618707	0.441841
6	3.830294	0.569312	1.377728
1	3.128329	0.889563	-0.566362
1	3.621698	0.382851	2.430887
6	5.197682	0.749780	0.989863
1	5.926327	0.741873	1.832159
8	5.631442	0.901138	-0.166704
6	-1.082687	2.192784	-1.632164
6	-1.946926	3.289738	-1.613789
6	-2.231554	3.933897	-0.406366
6	-1.637987	3.474874	0.772041
6	-0.772192	2.377683	0.746846
1	-0.854252	1.711246	-2.582532
1	-2.388131	3.646805	-2.541363

1	-2.897988	4.792454	-0.386942
1	-1.838932	3.978270	1.714671
1	-0.294607	2.049423	1.664935

$E_{(MeCN)}$ = -1248.928531
NImag = 0

65. **3b**-*c* conformer 2 (-1248.700582)

6	2.458960	-1.370035	1.627890
1	2.439812	-2.267285	1.004036
1	3.191704	-0.657745	1.243888
16	0.814796	-0.562302	1.610077
6	-0.103661	-1.973342	2.402847
1	0.022272	-2.904085	1.843561
1	-1.160472	-1.711714	2.459046
6	0.142199	-0.653135	-0.199255
1	0.952908	-1.207343	-0.680110
6	0.290978	0.826936	-0.697071
6	-0.861799	1.758990	-0.355724
1	0.290041	0.713908	-1.792523
6	1.635687	1.329432	-0.205218
6	-1.133100	-1.433028	-0.390631
1	0.303509	-2.074598	3.412279
1	2.677695	-1.636320	2.665913
6	-2.381809	-1.006420	0.095733
6	-3.530149	-1.765763	-0.133671
6	-3.456704	-2.960507	-0.857003
6	-2.224019	-3.395283	-1.349133
6	-1.073996	-2.638923	-1.111375
1	-2.460513	-0.077898	0.651613
1	-4.486383	-1.418953	0.249270
1	-4.354638	-3.545776	-1.037084
1	-2.154955	-4.319176	-1.917262
1	-0.118541	-2.981922	-1.503497
1	1.644934	2.257319	0.362466
6	2.827202	0.811816	-0.690730
6	4.144987	1.189755	-0.411719
1	2.763936	-0.061452	-1.349396
1	4.358363	2.091126	0.161984
6	5.249675	0.408945	-0.873583
1	6.252415	0.836832	-0.647203
8	5.193574	-0.682021	-1.475881
6	-1.801070	2.093601	-1.342658
6	-2.875705	2.942361	-1.064528
6	-3.033665	3.476023	0.216988
6	-2.100624	3.161663	1.209253
6	-1.024228	2.316727	0.923931
1	-1.688104	1.684794	-2.344435
1	-3.585892	3.188217	-1.850196

1	-3.867034	4.138256	0.437405
1	-2.202904	3.583255	2.206424
1	-0.298440	2.104656	1.703594

$E_{(MeCN)}$ = -1248.927469
NImag = 0

66. **3b**-R‡ (-1248.679240)

6	-0.129682	2.698281	-0.662884
6	-0.828285	1.633668	-0.068327
6	-2.231314	1.614393	-0.158176
6	-2.913957	2.626268	-0.837617
6	-2.210751	3.685188	-1.416681
6	-0.816156	3.719875	-1.323106
6	-0.159439	0.448398	0.596748
16	1.278298	1.082334	1.645264
6	0.441480	2.103413	2.913028
6	1.677634	-0.385575	2.656741
6	0.186527	-0.826455	-0.392036
6	-0.502822	-2.034786	0.128600
6	-1.840823	-2.263547	-0.140298
6	-2.719076	-3.202668	0.419093
6	-4.095594	-3.246421	0.054425
8	-4.694297	-2.492340	-0.741802
6	1.673706	-0.952365	-0.731042
6	2.411982	-2.102773	-0.411383
6	3.763106	-2.214141	-0.756975
6	4.404044	-1.182645	-1.447924
6	3.676985	-0.042116	-1.799092
6	2.329983	0.067553	-1.443413
1	-4.683732	-4.045240	0.564605
1	-2.368310	-3.918919	1.162622
1	-2.307366	-1.624337	-0.896483
1	-0.014679	-2.612562	0.916063
1	-0.831514	0.037492	1.353800
1	1.172825	2.355117	3.686076
1	0.088898	3.011308	2.421253
1	-0.400435	1.554220	3.341831
1	2.377412	-0.064759	3.432301
1	0.768080	-0.801545	3.095779
1	2.155096	-1.113847	2.000854
1	-0.322849	-0.512990	-1.311774
1	1.914955	-2.935401	0.075752
1	4.307868	-3.120138	-0.502222
1	5.450115	-1.275400	-1.728433
1	4.152006	0.755942	-2.364778
1	1.770578	0.944838	-1.757478
1	-2.790329	0.790895	0.278993
1	-3.996976	2.581012	-0.910674
1	-2.743030	4.475388	-1.939122
1	-0.258451	4.538821	-1.770187
1	0.956174	2.740207	-0.616666

$E_{(MeCN)}$ = -1248.918111
NImag = 1 (-22.3)

67. **3b**-*t* (-1248.723303) [$PCM_{(MeCN)}$/B3LYP/6-31+G* geometry]

6	-2.524248	1.151971	1.135524
6	-1.850216	0.944717	-0.080772
6	-2.564980	1.111457	-1.277315
6	-3.919204	1.468354	-1.263998
6	-4.579992	1.664882	-0.047966
6	-3.875309	1.507294	1.152923
6	-0.370699	0.562467	-0.124987
6	0.495280	1.506082	0.681828
6	1.429841	2.328499	0.135019
6	2.253547	3.281210	0.824063
6	3.139037	4.155464	0.198735
8	3.392311	4.290247	-1.053849
6	-0.098797	-0.885865	0.379878
6	1.312760	-1.377256	0.172670
6	1.924155	-1.340380	-1.091822
6	3.224334	-1.820983	-1.259764
6	3.932009	-2.336739	-0.167431
6	3.330883	-2.373664	1.094395
6	2.024753	-1.903770	1.261018
16	-1.261120	-2.133421	-0.546820
6	-0.569558	-3.762036	-0.104445
6	-2.807994	-2.205229	0.420579
1	-2.580667	-2.289860	1.486650
1	-3.382212	-1.303714	0.214522
1	-0.452002	-3.844750	0.978871
1	0.390044	-3.872422	-0.609405
1	-0.391869	-0.992413	1.432378
1	-0.052038	0.615478	-1.173700
1	-1.274999	-4.509985	-0.477785
1	-3.352254	-3.086832	0.069583
1	1.390388	-0.937620	-1.952887
1	3.687227	-1.788892	-2.245508
1	4.948179	-2.706637	-0.300737
1	3.875344	-2.770946	1.950432
1	1.557799	-1.936940	2.245991
1	0.318277	1.525874	1.760004
1	1.572255	2.280937	-0.948768
1	2.178184	3.349120	1.911251
1	3.693438	4.824709	0.892810
1	-2.056511	0.965482	-2.231354
1	-4.454027	1.593301	-2.205319

1	-5.633321	1.943095	-0.033300
1	-4.380207	1.661588	2.106345
1	-1.995202	1.035343	2.081040

$E_{(MeCN)}$ = -1248.934981
NImag = 0

68. **3b**-*t*‡ (-1242.412841) [HF/6-31+G* geometry]

6	2.650390	1.268230	-1.093110
6	1.976247	1.036283	0.107031
6	2.704961	1.107779	1.289718
6	4.067484	1.387207	1.281218
6	4.725830	1.600393	0.081558
6	4.007434	1.544783	-1.107603
6	0.486531	0.720900	0.139809
6	-0.365687	1.674064	-0.654502
6	-1.532625	2.178169	-0.162032
6	-2.473602	3.032182	-0.759025
6	-3.644259	3.402913	-0.062476
8	-3.997244	3.059354	1.061847
6	0.174022	-0.712240	-0.387522
6	-1.248629	-1.180278	-0.192756
6	-1.846231	-1.187041	1.064530
6	-3.155337	-1.611815	1.217745
6	-3.884371	-2.035087	0.115308
6	-3.297158	-2.030391	-1.139635
6	-1.984637	-1.607770	-1.290546
16	1.281299	-2.048963	0.498905
6	0.565710	-3.639645	0.021355
6	2.841786	-2.138967	-0.412255
1	2.653024	-2.159983	-1.476332
1	3.444306	-1.285058	-0.153386
1	0.456135	-3.700110	-1.051963
1	-0.395987	-3.739190	0.497813
1	0.469027	-0.807607	-1.422947
1	0.171882	0.754144	1.175605
1	1.233962	-4.412568	0.377346
1	3.340025	-3.047984	-0.102431
1	-1.308540	-0.836478	1.927542
1	-3.612732	-1.585794	2.189735
1	-4.906870	-2.344838	0.232611
1	-3.862009	-2.334914	-2.002118
1	-1.548073	-1.578505	-2.273566
1	-0.034883	1.924447	-1.649606
1	-1.802887	1.888550	0.842754
1	-2.321884	3.417481	-1.754166
1	-4.306663	4.078840	-0.621294
1	2.205042	0.962918	2.232080
1	4.605058	1.448128	2.210987

1	5.777548	1.824354	0.070305
1	4.503514	1.730411	-2.044001
1	2.111025	1.254325	-2.023076

$E_{(MeCN)}$ = -1248.929325
NImag = 0

69. **3b**-E‡ (-1242.411073) [HF/6-31+G* geometry]

16	1.357995	-2.190811	0.057962
6	1.240425	-2.239268	1.857222
6	0.493911	-3.715899	-0.374673
6	0.101195	-0.612979	-0.553338
6	0.612004	0.695854	0.063941
6	2.121133	0.874368	-0.019645
6	-0.170576	1.745076	-0.683830
1	1.693808	-1.339653	2.244311
1	1.799093	-3.096612	2.208724
1	0.209428	-2.312697	2.170509
1	1.073859	-4.550242	-0.002048
1	-0.502116	-3.727963	0.042004
1	0.441388	-3.776001	-1.452582
1	0.363538	-0.677427	-1.595634
1	0.332121	0.721276	1.109265
1	0.193843	2.015566	-1.661608
6	-1.307910	-1.057057	-0.314571
6	-1.934359	-0.937607	0.924346
6	-3.242801	-1.356691	1.095577
6	-3.946199	-1.904046	0.031820
6	-3.335424	-2.023801	-1.206710
6	-2.026075	-1.602211	-1.375672
1	-1.427128	-0.479506	1.752302
1	-3.720726	-1.227278	2.049221
1	-4.967483	-2.212426	0.163185
1	-3.880024	-2.424214	-2.042665
1	-1.571536	-1.671367	-2.348882
6	-1.293016	2.323583	-0.157349
6	-2.158474	3.277200	-0.699757
1	-1.579952	2.010873	0.835327
1	-1.986236	3.696959	-1.676987
6	-3.287661	3.713580	0.035946
1	-3.897344	4.470076	-0.476031
8	-3.649219	3.343848	1.146427
6	2.812301	0.781210	-1.227031
6	4.181032	0.985151	-1.282985
6	4.892412	1.292220	-0.130375
6	4.217152	1.399917	1.073782
6	2.844495	1.191671	1.124754
1	2.282479	0.569281	-2.139504
1	4.691674	0.913985	-2.227119

1	5.954241	1.455818	-0.175384
1	4.751343	1.654348	1.972161
1	2.330155	1.307764	2.063933

$E_{(MeCN)}$ = -1248.928121
NImag = 1 (-288.8)

70. **3b**-PC (-1248.773934)

16	-2.524157	2.689118	-1.510667
6	-2.942055	3.093052	0.221807
6	-1.313975	4.015502	-1.850457
6	0.247324	0.050911	-0.007114
6	-0.094326	-1.310916	0.520114
6	-1.467936	-1.894082	0.516021
6	0.714538	-1.175094	-0.794582
1	-3.667959	2.349255	0.561897
1	-3.395186	4.087160	0.294495
1	-2.057216	3.042851	0.864480
1	-1.776935	5.003168	-1.754999
1	-0.451306	3.945187	-1.180209
1	-0.973135	3.886250	-2.881642
1	-0.567944	0.579456	-0.502563
1	0.514647	-1.643285	1.358809
6	1.199440	0.965352	0.709193
6	1.188085	1.079330	2.106361
6	2.042705	1.973284	2.759373
6	2.923199	2.767776	2.021591
6	2.942894	2.663661	0.626760
6	2.087199	1.771414	-0.021918
1	0.502375	0.467047	2.687152
1	2.020386	2.045710	3.843956
1	3.592444	3.458731	2.527702
1	3.630607	3.271930	0.044452
1	2.113011	1.687708	-1.106181
6	2.113277	-1.601808	-0.813146
6	2.707808	-2.253853	-1.836485
1	2.720640	-1.382815	0.065124
1	2.155569	-2.495517	-2.744112
6	4.117419	-2.672101	-1.786942
1	4.485145	-3.191857	-2.697402
8	4.878103	-2.491714	-0.846072
6	-2.470604	-1.473193	-0.374189
6	-3.737725	-2.059593	-0.351710
6	-4.031733	-3.076788	0.561487
6	-3.044291	-3.502606	1.453405
6	-1.776415	-2.917093	1.427707
1	-2.271653	-0.677312	-1.087601
1	-4.497824	-1.717607	-1.049904
1	-5.019128	-3.530809	0.577598
1	-3.258118	-4.292049	2.169714
1	-1.013010	-3.258145	2.124062
1	0.147325	-1.386178	-1.699247

$E_{(MeCN)}$ = -1248.976282
NImag = 0

HF/6-31+G* Optimized Geometries of the TSs and Intermediates Along the Reaction Profiles 2a and 2b (Figure S3)

71. **2a**-A-$c^{\ddagger}$ (-1242.407951)

6	-4.082736	-1.271200	0.125360
6	-3.350062	-0.149903	-0.269984
6	-3.986894	1.090310	-0.253847
6	-5.303017	1.215284	0.166327
6	-6.013083	0.096084	0.571157
6	-5.396483	-1.148469	0.544820
6	-1.939681	-0.222953	-0.709940
6	-1.076858	-1.198531	-0.448423
6	0.307823	-1.217002	-0.959848
6	0.905200	-2.443511	-1.283561
6	2.065364	-2.487314	-2.099410
8	2.731869	-1.531534	-2.463551
6	1.234291	-0.144800	0.676754
16	2.746279	-0.996523	1.060293
6	2.151824	-2.451479	1.932853
6	1.472695	1.248804	0.217262
6	2.309720	1.533539	-0.869790
6	2.478418	2.838247	-1.307706
6	1.801767	3.885538	-0.696835
6	0.951530	3.613249	0.364621
6	0.795241	2.312518	0.820539
6	3.556708	-0.122932	2.422377
1	1.535319	-2.152335	2.770289
1	1.583480	-3.037006	1.229124
1	2.872434	0.004673	3.250188
1	3.867537	0.842806	2.050624
1	0.602414	-0.185794	1.555026
1	0.448368	-3.370843	-0.978749
1	4.426916	-0.689621	2.730363
1	3.007236	-3.017008	2.277034
1	2.375606	-3.490585	-2.415278
1	-1.374163	-2.048054	0.144182
1	-1.595957	0.621067	-1.285463
1	0.580944	-0.387044	-1.581325
1	-3.634231	-2.247047	0.086088
1	-5.944261	-2.025938	0.840391
1	-7.035170	0.187927	0.892909

1	-5.770963	2.183849	0.173744
1	-3.445116	1.965745	-0.567809
1	0.138952	2.119438	1.651757
1	0.414859	4.412719	0.845271
1	1.929258	4.894301	-1.047330
1	3.127488	3.031915	-2.143493
1	2.803020	0.730588	-1.390189

$E_{(MeCN)}$ = -1248.905191
NImag = 1 (-415.5)

73. **2a**-A-$t^{\ddagger}$ (-1242.409564)

6	-3.462664	0.451036	0.400801
6	-3.039540	-0.816065	-0.007868
6	-3.978084	-1.666478	-0.590018
6	-5.301204	-1.278379	-0.743381
6	-5.709881	-0.023276	-0.322186
6	-4.782483	0.839617	0.248733
6	-1.644985	-1.284683	0.142927
6	-0.715750	-0.779209	0.946062
6	0.642331	-1.343676	1.063407
6	1.824415	-0.019764	-0.109364
16	2.090895	-0.490987	-1.806474
6	2.483257	-2.250717	-1.709519
6	1.398805	1.396590	0.026274
6	0.401804	1.981030	-0.765727
6	-0.012774	3.284111	-0.547444
6	0.537227	4.039344	0.480551
6	1.514510	3.470712	1.282072
6	1.946689	2.171978	1.052756
6	3.702790	0.172798	-2.297312
6	1.283667	-1.380931	2.308748
6	2.479677	-2.120276	2.444042
8	3.078823	-2.688019	1.534186
1	3.046516	-2.457272	-0.809339
1	1.554343	-2.800655	-1.693737
1	4.462309	-0.166371	-1.605967
1	3.629724	1.250624	-2.269595
1	2.741677	-0.230854	0.415003
1	0.920140	-0.797425	3.135788
1	3.931278	-0.152667	-3.304473
1	3.035604	-2.514306	-2.601654
1	2.903774	-2.166314	3.451608
1	-0.937214	0.056314	1.586302
1	-1.391430	-2.147357	-0.454057
1	0.840394	-2.178054	0.421689
1	-2.758468	1.141967	0.826363
1	-5.087401	1.819965	0.569981
1	-6.734130	0.282699	-0.440053

1	-6.007909	-1.955703	-1.189375
1	-3.673223	-2.645725	-0.917106
1	2.713916	1.751272	1.677813
1	1.952222	4.039497	2.083725
1	0.209675	5.049378	0.650781
1	-0.777184	3.706851	-1.175961
1	-0.066371	1.411497	-1.548952

$E_{(MeCN)}$ = -1248.903869
NImag = 1 (-445.2)

74. **2a**-*c* (-1242.438100)

6	-2.409922	1.428589	0.974113
6	-1.655681	1.141295	-0.164768
6	-1.335327	2.167304	-1.046827
6	-1.762416	3.466868	-0.806699
6	-2.522760	3.745615	0.317561
6	-2.844187	2.724883	1.203911
6	-1.158667	-0.262345	-0.433830
16	-2.595491	-1.403322	-0.767287
6	-3.603188	-0.436902	-1.919790
6	-0.268022	-0.893882	0.707318
6	-0.695895	-2.282175	1.122393
6	-1.738909	-2.401434	2.023553
8	-2.504819	-1.486706	2.379370
6	1.167332	-0.849276	0.246467
6	2.081185	-0.004049	0.701929
6	3.501639	0.061669	0.283693
6	4.190129	1.267824	0.405168
6	5.514804	1.380212	0.009719
6	6.182386	0.281135	-0.508336
6	5.514291	-0.931097	-0.618331
6	4.191284	-1.041226	-0.222215
6	-1.912779	-2.585339	-1.947530
1	-1.446926	-2.068867	-2.776647
1	-1.200630	-3.192640	-1.414566
1	-3.010363	-0.024305	-2.724517
1	-4.082351	0.357827	-1.369498
1	-0.622414	-0.267070	-1.374791
1	-0.009003	-3.102050	0.989533
1	-4.358676	-1.102651	-2.317216
1	-2.727849	-3.201903	-2.304247
1	-1.915617	-3.407714	2.420631
1	1.439067	-1.569493	-0.512002
1	1.785420	0.724544	1.439982
1	-0.378887	-0.227521	1.553372
1	3.700994	-1.995658	-0.285092
1	6.028472	-1.795455	-1.000491
1	7.211117	0.363106	-0.811162

1	6.023154	2.323075	0.109207
1	3.682244	2.127426	0.807490
1	-0.737907	1.960765	-1.918533
1	-1.499170	4.252282	-1.492667
1	-2.857367	4.750172	0.506841
1	-3.426674	2.938528	2.082207
1	-2.642009	0.638372	1.668808

$E_{(MeCN)}$ = -1248.930456
NImag = 0

75. **2a**-R‡ (-1242.430805)

6	0.386477	1.939868	-0.636921
6	1.233709	1.426214	0.344761
6	1.598987	2.246567	1.406328
6	1.128836	3.551242	1.492849
6	0.295580	4.053868	0.507966
6	-0.072768	3.243717	-0.559085
6	1.761586	0.005866	0.310550
16	2.703753	-0.231233	-1.278024
6	3.862735	1.149755	-1.326657
6	0.748386	-1.213760	0.467432
6	1.113983	-2.072237	1.649814
6	1.773520	-3.259763	1.469866
8	2.232600	-3.722519	0.392330
6	-0.688598	-0.760637	0.540517
6	-1.625548	-1.119951	-0.325506
6	-3.062817	-0.766679	-0.266352
6	-3.824280	-0.832102	-1.432518
6	-5.169842	-0.494055	-1.433340
6	-5.785915	-0.088765	-0.260003
6	-5.043929	-0.034044	0.912987
6	-3.701336	-0.373148	0.911646
6	3.816849	-1.614461	-0.930219
1	4.514182	-1.317068	-0.158865
1	3.224924	-2.469378	-0.591612
1	4.391035	1.227686	-0.386663
1	3.316691	2.058587	-1.525759
1	2.516719	-0.105450	1.072949
1	0.733380	-1.804856	2.621895
1	4.560253	0.957476	-2.131044
1	4.337423	-1.836636	-1.852318
1	1.917699	-3.856165	2.375609
1	-0.948197	-0.146631	1.387448
1	-1.340925	-1.726465	-1.171347
1	0.846649	-1.839904	-0.412880
1	-3.154277	-0.351450	1.836221
1	-5.515666	0.261502	1.833688
1	-6.829972	0.169465	-0.254564
1	-5.733906	-0.551749	-2.347682
1	-3.358801	-1.150469	-2.349663
1	2.243379	1.864710	2.178921
1	1.415061	4.166787	2.326746
1	-0.069536	5.063252	0.570468
1	-0.728882	3.622371	-1.322050
1	0.068217	1.319293	-1.454444

$E_{(MeCN)}$ = -1248.926923
NImag = 1 (-26.7)

76. **2a**-*t*‡ (-1242.439071)

6	0.601246	1.896171	-0.769993
6	1.531266	1.240275	0.035530
6	2.359266	2.000625	0.855959
6	2.259535	3.385225	0.875865
6	1.337648	4.028083	0.065196
6	0.509206	3.279232	-0.759440
6	1.676539	-0.265657	0.076663
16	1.880897	-0.890735	-1.682250
6	3.477442	-0.176712	-2.126461
6	0.597436	-1.106733	0.842317
6	1.091865	-1.246587	2.264104
6	2.264222	-1.915689	2.481955
8	3.023652	-2.389794	1.587930
6	-0.792273	-0.534941	0.753618
6	-1.809325	-1.131574	0.146549
6	-3.202777	-0.635203	0.056341
6	-4.041663	-1.152102	-0.929499
6	-5.349459	-0.709114	-1.066338
6	-5.848129	0.259441	-0.210223
6	-5.028104	0.773539	0.786353
6	-3.723686	0.329428	0.921445
6	2.342342	-2.634660	-1.461746
1	2.822398	-2.755901	-0.496526
1	1.440549	-3.225093	-1.513360
1	4.214736	-0.447466	-1.383190
1	3.365391	0.895742	-2.175730
1	2.624210	-0.538037	0.506647
1	0.487813	-0.887807	3.077541
1	3.758968	-0.559582	-3.097886
1	2.990196	-2.897204	-2.287528
1	2.573702	-2.029743	3.523839
1	-0.943110	0.409391	1.248689
1	-1.634878	-2.075639	-0.346907
1	0.578189	-2.090986	0.382875
1	-3.116159	0.723062	1.715399
1	-5.409465	1.514309	1.466906
1	-6.862434	0.602965	-0.309210
1	-5.975198	-1.122814	-1.837472
1	-3.667338	-1.907547	-1.599126

1	3.069721	1.506529	1.493542
1	2.901152	3.955588	1.523382
1	1.261519	5.100726	0.076601
1	-0.214552	3.768649	-1.386411
1	-0.064551	1.332690	-1.398688

$E_{(MeCN)}$ = -1248.926693
NImag = 1

2a-E‡ (See Structure No. 39 above)

77. **2a**-PC (-1242.529612)

6	-4.237452	-2.365980	-0.093810
6	-3.480237	-1.195913	-0.083127
6	-4.138809	0.017455	-0.291190
6	-5.510404	0.056319	-0.477219
6	-6.254852	-1.116255	-0.470164
6	-5.611447	-2.329009	-0.280920
6	-2.019218	-1.288294	0.137287
6	-1.225772	-0.319555	0.576102
6	0.234588	-0.488590	0.768773
6	0.898897	0.152019	1.983113
6	1.915759	-0.631738	2.724161
8	2.731468	-1.336409	2.210037
6	1.205687	0.632246	0.587822
16	4.327495	-1.608836	-1.688386
6	5.537943	-1.022098	-0.478125
6	0.798760	2.000378	0.120483
6	0.847228	3.110518	0.954357
6	0.505839	4.371571	0.480455
6	0.114603	4.537341	-0.837849
6	0.069180	3.434856	-1.681768
6	0.408518	2.179009	-1.205702
6	3.878597	-3.189691	-0.930866
1	0.619102	-1.461463	0.516920
1	2.165232	0.308807	0.221213
1	6.394551	-1.683947	-0.434753
1	5.090174	-0.942257	0.503859
1	5.871950	-0.042947	-0.797350
1	3.480492	-3.037839	0.063664
1	3.119185	-3.646301	-1.553185
1	4.733569	-3.853559	-0.884914
1	0.371004	1.329277	-1.864580
1	-0.230219	3.553583	-2.708048
1	-0.149677	5.512557	-1.206356
1	0.550054	5.219293	1.141206
1	1.158431	2.997739	1.977752
1	1.884477	-0.541870	3.813454
1	-1.633491	0.647093	0.817482
1	-1.586151	-2.254403	-0.069410
1	-3.578700	0.934097	-0.326718
1	-5.997865	1.001591	-0.638539
1	-7.319418	-1.083384	-0.618959
1	-6.174951	-3.245249	-0.279580
1	-3.748760	-3.313782	0.053073
1	0.264911	0.768084	2.596775

$E_{(MeCN)}$ = -1248.979481
NImag = 0

78. **2b**-A-*c*‡ (-1242.413579)

6	4.233189	-1.592916	-0.661880
6	3.264043	-0.761006	-0.103745
6	3.654772	0.510434	0.323779
6	4.971605	0.921507	0.211751
6	5.929280	0.076986	-0.336472
6	5.553647	-1.182269	-0.775196
6	1.873738	-1.253811	0.002079
6	0.905628	-0.754493	0.762005
6	-0.445010	-1.345386	0.844434
6	-1.128234	-1.318092	2.063974
6	-2.243360	-2.156993	2.284555
8	-2.781030	-2.883930	1.454742
6	-1.355680	-0.068419	-0.650636
16	-3.039757	-0.563773	-0.926591
6	-3.611589	0.312108	-2.404788
6	-1.264901	1.340078	-0.193151
6	-2.040729	1.841869	0.858585
6	-1.876313	3.143871	1.308640
6	-0.927790	3.977567	0.735615
6	-0.144264	3.490916	-0.302019
6	-0.314588	2.195609	-0.762940
6	-2.915696	-2.238664	-1.569817
1	-2.158541	-2.281493	-2.341747
1	-2.684797	-2.878610	-0.732586
1	-4.617765	-0.013233	-2.638988
1	-2.947979	0.117577	-3.236784
1	-0.799706	-0.244680	-1.563356
1	-0.815376	-0.650495	2.846890
1	-3.615942	1.368503	-2.177293
1	-3.882119	-2.505630	-1.976488
1	-2.654705	-2.139146	3.298345
1	-0.594813	-2.213557	0.232309
1	1.085517	0.094477	1.397337
1	1.656974	-2.127595	-0.592775
1	3.953999	-2.575046	-1.002731
1	6.283933	-1.845599	-1.203865
1	6.951288	0.400354	-0.423199
1	5.251061	1.904724	0.547031
1	2.928149	1.187084	0.734472

1	0.300051	1.838349	-1.570916
1	0.596154	4.123107	-0.760640
1	-0.802110	4.985577	1.088512
1	-2.488268	3.502314	2.117913
1	-2.767149	1.211438	1.337451

$E_{(MeCN)}$ = -1248.908826
NImag = 1 (-428.4)

79. **2b**-A-$t^{\ddagger}$ (-1242.394853)

6	-4.138363	0.133021	1.465460
6	-3.477453	-0.520547	0.425376
6	-4.217922	-0.870331	-0.706394
6	-5.562827	-0.552758	-0.800834
6	-6.203493	0.113099	0.236077
6	-5.485538	0.450598	1.372739
6	-2.032990	-0.813745	0.562655
6	-1.175685	-1.032787	-0.428153
6	0.251107	-1.365690	-0.226269
6	0.835164	-2.320889	-1.068113
6	1.909309	-3.143889	-0.624724
8	2.466325	-3.111733	0.456101
6	1.202078	0.435313	-0.617684
16	0.459062	2.002658	-0.084174
6	1.537392	3.359564	-0.614953
6	2.583690	0.347828	-0.052188
6	2.819189	0.412481	1.324174
6	4.097368	0.279778	1.835139
6	5.173783	0.060122	0.985164
6	4.953925	-0.018547	-0.379215
6	3.673402	0.134598	-0.893139
6	-0.918729	2.262295	-1.214889
1	-0.587814	2.123751	-2.235392
1	-1.699032	1.561106	-0.972734
1	1.057968	4.300016	-0.373231
1	1.725799	3.289351	-1.677641
1	1.214919	0.461164	-1.700027
1	0.439163	-2.485673	-2.056848
1	2.466091	3.271505	-0.071482
1	-1.280447	3.271592	-1.072150
1	2.229114	-3.898479	-1.355121
1	0.566553	-1.404639	0.799880
1	-1.511431	-1.018723	-1.452643
1	-1.661703	-0.829306	1.575416
1	-3.592872	0.394934	2.355879
1	-5.971874	0.955812	2.188490
1	-7.249379	0.352225	0.162811
1	-6.115344	-0.838428	-1.678483
1	-3.750697	-1.416446	-1.505413
1	3.518425	0.069198	-1.955567
1	5.776151	-0.202013	-1.048260
1	6.164516	-0.061763	1.384874
1	4.251417	0.321024	2.898910
1	1.994443	0.538021	2.005312

$E_{(MeCN)}$ = -1248.898249
NImag = 1 (-442.6)

80. **2b**-*c* (-1242.444185)

6	4.265869	-1.125984	-1.067840
6	3.399395	-0.641113	-0.089654
6	3.901098	0.278003	0.834140
6	5.214325	0.710852	0.763105
6	6.062286	0.230021	-0.226642
6	5.582495	-0.694250	-1.140616
6	1.998481	-1.123992	-0.068241
6	0.967394	-0.540175	0.526687
6	-0.438171	-1.096126	0.534894
6	-0.986361	-1.226439	1.933687
6	-1.967335	-2.140994	2.180555
8	-2.570780	-2.822241	1.304380
6	-1.282545	-0.218636	-0.452651
16	-3.012267	-0.882759	-0.636351
6	-3.613538	0.145168	-1.996284
6	-1.377823	1.261406	-0.130388
6	-2.037152	1.741221	1.000323
6	-2.082994	3.103524	1.258244
6	-1.467599	4.004013	0.400342
6	-0.804970	3.535005	-0.723188
6	-0.766820	2.173224	-0.986577
6	-2.807117	-2.441195	-1.521654
1	-2.157109	-2.300551	-2.375250
1	-2.420892	-3.145358	-0.803829
1	-4.567236	-0.259643	-2.309673
1	-2.921688	0.144607	-2.828072
1	-0.863391	-0.325098	-1.447212
1	-0.503624	-0.701374	2.739017
1	-3.755268	1.151797	-1.633986
1	-3.792252	-2.749952	-1.845792
1	-2.260433	-2.278448	3.224503
1	-0.404918	-2.082835	0.081260
1	1.106586	0.387004	1.057236
1	1.830566	-2.046299	-0.602910
1	3.906173	-1.847097	-1.781794
1	6.229799	-1.082277	-1.907306
1	7.083250	0.564487	-0.276064
1	5.580458	1.416409	1.488041
1	3.270892	0.644057	1.623645
1	-0.241770	1.820691	-1.857373
1	-0.318168	4.221933	-1.392201

1	-1.502294	5.058771	0.607246
1	-2.594313	3.458477	2.135160
1	-2.495349	1.051571	1.682499

$E_{(MeCN)}$ = -1248.933973
NImag = 0

81. **2b**-R‡ (-1242.417996)

6	4.675760	0.216967	-0.860856
6	3.699705	-0.299827	-0.009663
6	4.084251	-0.666434	1.282018
6	5.389585	-0.493248	1.710534
6	6.346935	0.040027	0.856875
6	5.984570	0.389842	-0.434070
6	2.312306	-0.442480	-0.508980
6	1.211862	-0.534991	0.225074
6	-0.181196	-0.762960	-0.316203
6	-0.634403	-2.166299	-0.031437
6	-1.258440	-2.869521	-1.033960
8	-1.620229	-2.425717	-2.147634
6	-1.141741	0.358682	0.253577
16	-1.205155	1.774437	-0.996275
6	-2.174816	3.065852	-0.192214
6	-2.590905	0.030658	0.535476
6	-3.413182	-0.549268	-0.428329
6	-4.749129	-0.782717	-0.142177
6	-5.274523	-0.456420	1.101605
6	-4.455872	0.104336	2.068816
6	-3.120237	0.350237	1.781065
6	0.425980	2.547811	-0.987778
1	0.751868	2.743728	0.023641
1	1.120238	1.883594	-1.473578
1	-2.130965	3.945767	-0.820324
1	-1.778342	3.283998	0.789627
1	-0.709278	0.814434	1.136499
1	-0.351894	-2.640710	0.892561
1	-3.194170	2.722146	-0.115839
1	0.345659	3.470119	-1.548003
1	-1.463441	-3.922279	-0.810355
1	-0.172682	-0.672081	-1.398098
1	1.290817	-0.512473	1.302456
1	2.216990	-0.481117	-1.583848
1	4.410144	0.483549	-1.869758
1	6.717958	0.791136	-1.111128
1	7.361407	0.166772	1.190509
1	5.664288	-0.788737	2.707845
1	3.368617	-1.111933	1.948444
1	-2.488748	0.777478	2.542028
1	-4.848067	0.344776	3.040985

1	-6.310011	-0.650864	1.318138
1	-5.372665	-1.243901	-0.886670
1	-3.002479	-0.870156	-1.369918

$E_{(MeCN)}$ = -1248.922850
NImag = 1 (-21.4)

82. **2b**-*t* (-1242.422495)

6	-4.350623	-0.250716	-1.235842
6	-3.571336	0.363412	-0.255588
6	-4.188816	0.732456	0.940930
6	-5.531811	0.468519	1.156827
6	-6.291173	-0.160589	0.179245
6	-5.695352	-0.514746	-1.021567
6	-2.132409	0.601470	-0.518968
6	-1.176177	0.695626	0.396150
6	0.273708	0.994850	0.107313
6	0.749020	2.217103	0.840501
6	1.433296	3.201531	0.152736
8	1.791896	3.178181	-1.038408
6	1.177009	-0.181594	0.528993
16	0.535029	-1.790360	-0.472709
6	1.891924	-2.982429	-0.507355
6	2.658059	-0.093643	0.286357
6	3.184688	0.479467	-0.867082
6	4.557996	0.493677	-1.067891
6	5.414635	-0.052729	-0.124734
6	4.896832	-0.608164	1.037683
6	3.526790	-0.626822	1.237121
6	-0.597636	-2.638632	0.652321
1	-0.149648	-2.738184	1.631856
1	-1.507931	-2.064070	0.709345
1	1.518798	-3.881358	-0.980673
1	2.246202	-3.198945	0.489507
1	0.976521	-0.479245	1.548754
1	0.443951	2.369151	1.862620
1	2.692520	-2.565343	-1.097872
1	-0.810668	-3.616379	0.241390
1	1.678050	4.090848	0.745590
1	0.398766	1.170752	-0.953610
1	-1.429974	0.595751	1.442116
1	-1.863632	0.699265	-1.559134
1	-3.900469	-0.522301	-2.175490
1	-6.275618	-0.990140	-1.792646
1	-7.335084	-0.357568	0.346561
1	-5.989845	0.768745	2.082756
1	-3.626200	1.253201	1.694180
1	3.133294	-1.038893	2.151356
1	5.554699	-1.010428	1.787389

1	6.478215	-0.027638	-0.282599
1	4.954054	0.960223	-1.951373
1	2.546621	0.974585	-1.572315

$E_{(MeCN)}$ = -1248.926685
NImag = 0

83. **2b**-$E^{‡}$ (-1242.422506)

6	-4.346859	-0.238992	-1.249808
6	-3.570194	0.367657	-0.263040
6	-4.190605	0.725947	0.935355
6	-5.533688	0.459106	1.146194
6	-6.290528	-0.162477	0.161726
6	-5.691823	-0.506165	-1.040547
6	-2.131180	0.608582	-0.522896
6	-1.178002	0.718283	0.393430
6	0.271531	1.016823	0.104247
6	0.754866	2.230001	0.847922
6	1.467586	3.206403	0.175307
8	1.844185	3.181175	-1.008917
6	1.178251	-0.144571	0.539026
16	0.511795	-1.800893	-0.454486
6	1.872899	-2.987425	-0.504431
6	2.654676	-0.081949	0.282062
6	3.180064	0.469293	-0.882727
6	4.551537	0.459291	-1.095634
6	5.407425	-0.089925	-0.153559
6	4.891393	-0.624778	1.019541
6	3.523399	-0.619283	1.231097
6	-0.595387	-2.639918	0.701902
1	-0.112308	-2.766061	1.661665
1	-1.487708	-2.043370	0.804224
1	1.497421	-3.895857	-0.957444
1	2.251599	-3.188627	0.486719
1	0.974796	-0.442363	1.557366
1	0.433199	2.384784	1.864340
1	2.658130	-2.573360	-1.117636
1	-0.852397	-3.605554	0.287452
1	1.717086	4.089083	0.775908
1	0.400359	1.193063	-0.955968
1	-1.433122	0.631659	1.440044
1	-1.859024	0.692221	-1.563351
1	-3.894395	-0.503119	-2.190407
1	-6.269815	-0.975941	-1.816743
1	-7.334549	-0.361945	0.325334
1	-5.993819	0.750886	2.073771
1	-3.630597	1.240622	1.694666
1	3.131016	-1.015470	2.152739
1	5.549603	-1.029620	1.767522
1	6.469823	-0.083672	-0.320995
1	4.947380	0.908700	-1.988036
1	2.542958	0.963403	-1.589048

$E_{(MeCN)}$ = -1248.926404
NImag = 1 (-99.1)

84. **2b**-PC (-1242.525491)

16	-0.575499	3.413476	-0.544075
6	-0.028362	3.150328	1.160129
6	0.223291	4.996833	-0.898467
6	1.537287	-0.421099	-0.675257
6	0.438521	-1.393965	-0.421119
6	1.226188	-1.497622	-1.707222
6	2.133740	-2.659432	-1.902162
8	2.501572	-3.390913	-1.037007
1	-0.433891	2.203575	1.491107
1	-0.400691	3.932642	1.810057
1	1.051882	3.106412	1.220933
1	-0.129926	5.768721	-0.225827
1	1.300580	4.915723	-0.822713
1	-0.035626	5.274041	-1.912191
1	1.207703	0.553200	-0.997497
1	0.661619	-2.185274	0.272729
1	0.760101	-1.148181	-2.613359
6	2.814180	-0.375018	0.113718
6	2.864591	-0.735001	1.453605
6	4.049355	-0.632988	2.171775
6	5.199632	-0.165219	1.558404
6	5.158881	0.203362	0.220024
6	3.975515	0.100137	-0.492255
1	1.979834	-1.098335	1.943914
1	4.069967	-0.921716	3.207759
1	6.117835	-0.089519	2.113316
1	6.046524	0.567266	-0.266710
1	3.952655	0.387736	-1.529880
1	2.465301	-2.821537	-2.931954
6	-0.979116	-0.957006	-0.455955
6	-1.936238	-1.501807	0.283927
1	-1.208997	-0.152498	-1.136140
1	-1.677033	-2.325734	0.930180
6	-3.365831	-1.116304	0.304320
6	-3.822410	0.130633	-0.127646
6	-5.172114	0.438842	-0.101375
6	-6.096665	-0.486774	0.365098
6	-5.655595	-1.722721	0.810434
6	-4.303120	-2.030143	0.783071
1	-3.125135	0.872486	-0.471676
1	-5.501274	1.406596	-0.436355
1	-7.143907	-0.243051	0.387570
1	-6.359993	-2.447204	1.179313

1	-3.972495	-2.993875	1.130381

$E_{(MeCN)}$ = -1248.976052
NImag = 0

II. Addition to Enone

1,2- Addition (Pathway 4)

85. **4a**-A-*c*‡ (-1018.858396)

6	2.440881	-0.281037	-1.340419
6	1.468947	-0.170333	-0.326288
6	1.883299	-0.341054	1.010785
6	3.224534	-0.590089	1.312796
6	4.179179	-0.685223	0.295564
6	3.778742	-0.539523	-1.036370
6	0.040311	0.054325	-0.681320
6	-1.165736	-1.236581	0.157141
6	-2.472696	-0.840299	-0.518069
6	-3.588754	-0.561905	0.167065
6	-4.922743	-0.223018	-0.436932
16	-0.625788	1.688879	-0.290798
6	-0.767812	1.763313	1.526771
6	0.698437	2.928855	-0.560873
8	-1.099128	-1.138981	1.435722
6	-0.589892	-2.527910	-0.459899
1	1.616904	2.610075	-0.062606
1	0.863106	3.015133	-1.637309
1	0.217270	1.918996	1.972117
1	-1.174270	0.783335	1.825437
1	-0.132781	-0.020878	-1.759293
1	-1.440424	2.591007	1.763782
1	0.348843	3.885245	-0.160422
1	-1.240814	-3.355054	-0.149754
1	-0.555141	-2.510062	-1.557016
1	0.412764	-2.719894	-0.068398
1	-2.493611	-0.845227	-1.611205
1	-3.527053	-0.603994	1.255261
1	-4.881655	-0.202179	-1.532450
1	-5.687398	-0.955017	-0.140553
1	-5.282315	0.757327	-0.091759
1	1.133493	-0.349664	1.794784
1	3.520752	-0.730668	2.349709
1	5.220748	-0.882476	0.536446
1	4.507683	-0.624240	-1.838942
1	2.139349	-0.169112	-2.380538

$E_{(MeCN)}$ = -1019.029911
NImag = 1 (-223.2)

86. **4a**-A-*t*‡ (-1018.841450)

6	-1.636318	2.925699	-0.630543
16	0.007977	2.118281	-0.421137
6	-0.105905	0.663346	0.758384
6	1.462052	-0.099730	1.274585
6	2.362444	-0.216123	0.039296
6	2.818211	-1.390044	-0.412668
6	3.785344	-1.583252	-1.547396
6	0.145547	1.365777	-2.073242
6	-1.186307	-0.301508	0.362579
8	1.087514	-1.191189	1.841064
6	2.052671	0.984665	2.220205
1	-2.395212	2.167113	-0.837270
1	-1.863626	3.444269	0.303424
1	0.239812	2.176879	-2.799400
1	-0.733678	0.751836	-2.280040
1	-0.386205	1.187238	1.678721
1	1.043582	0.747087	-2.076812
1	-1.571774	3.650970	-1.447662
1	3.026304	0.628453	2.577024
1	2.202995	1.962575	1.738612
1	1.399695	1.103545	3.092022
1	2.724522	0.715680	-0.410950
1	2.464279	-2.280725	0.108715
1	4.085568	-0.629582	-1.999457
1	4.696726	-2.093271	-1.204546
1	3.357640	-2.216518	-2.338627
6	-2.472813	-0.193090	0.917536
6	-3.488869	-1.088508	0.571981
6	-3.230504	-2.116634	-0.337681
6	-1.949960	-2.247992	-0.884626
6	-0.937018	-1.353094	-0.535917
1	-2.673714	0.586886	1.649827
1	-4.474120	-0.989093	1.021023
1	-4.014712	-2.820546	-0.605128
1	-1.733140	-3.063851	-1.569909
1	0.065870	-1.488989	-0.924844

$E_{(MeCN)}$ = -1019.018819
NImag = 1 (-254.1)

87. **4a**-*c* (-1018.868462)

6	2.248921	-0.269096	-1.475723
6	1.400502	-0.299004	-0.355469
6	1.969538	-0.563499	0.905825
6	3.340691	-0.790056	1.032099
6	4.173129	-0.754806	-0.092078
6	3.622375	-0.495830	-1.348945

6	-0.075021	-0.083340	-0.545397
6	-1.104093	-0.959867	0.276056
6	-2.423736	-0.971874	-0.514654
6	-3.581799	-0.525689	-0.019761
6	-4.908946	-0.564934	-0.724997
16	-0.712708	1.559752	0.164157
6	0.273168	2.117571	1.587956
6	0.080709	2.704903	-1.077573
8	-1.177581	-0.291703	1.472229
6	-0.655884	-2.435763	0.415469
1	1.161457	2.548937	-1.149396
1	-0.386067	2.521762	-2.049342
1	1.327730	1.868811	1.451578
1	-0.136929	1.609387	2.458358
1	-0.285070	-0.006421	-1.621067
1	0.150045	3.203179	1.652893
1	-0.128829	3.734723	-0.774817
1	-1.425560	-2.965820	0.985336
1	-0.545486	-2.932078	-0.558692
1	0.288749	-2.521633	0.957601
1	-2.392651	-1.417773	-1.514549
1	-3.556941	-0.110579	0.988471
1	-4.826854	-0.997518	-1.729495
1	-5.639736	-1.160260	-0.159224
1	-5.338758	0.442421	-0.822974
1	1.316380	-0.604719	1.772159
1	3.760411	-1.000759	2.012718
1	5.240523	-0.932783	0.011543
1	4.257071	-0.473692	-2.231279
1	1.827160	-0.079884	-2.461021

$E_{(MeCN)}$ = -1019.037164
NImag = 0

88. **4a**-R‡ (-1014.030182) [HF/6-31+G* geometry]

6	-2.562004	-0.039766	0.850714
6	-1.329293	-0.286882	0.254913
6	-1.292369	-1.090247	-0.885758
6	-2.463506	-1.589983	-1.429035
6	-3.690607	-1.320969	-0.833802
6	-3.738243	-0.550557	0.314833
6	-0.078311	0.284522	0.870305
6	1.227539	-0.787710	1.050548
6	2.431217	-0.277907	0.236173
6	3.014032	-1.014529	-0.695166
6	4.252669	-0.636565	-1.460417
16	0.396195	1.907396	0.051186
6	0.404908	1.645220	-1.732034
6	-1.037404	2.989984	0.215478
8	0.828942	-1.976877	0.734410
6	1.595001	-0.636038	2.547771
1	-1.918733	2.523011	-0.198149
1	-1.181911	3.193744	1.267281
1	-0.562326	1.300092	-2.063751
1	1.166013	0.913260	-1.949429
1	-0.323671	0.667587	1.853810
1	0.655531	2.591164	-2.193887
1	-0.817841	3.916408	-0.299334
1	2.435501	-1.288898	2.755229
1	1.870313	0.381107	2.833751
1	0.759452	-0.962705	3.159587
1	2.876923	0.671630	0.509693
1	2.576787	-1.978261	-0.897645
1	4.621138	0.345310	-1.178789
1	5.048125	-1.356185	-1.282817
1	4.068794	-0.635082	-2.533238
1	-0.345576	-1.360792	-1.306445
1	-2.417213	-2.216170	-2.302346
1	-4.595185	-1.724971	-1.252978
1	-4.677935	-0.354228	0.800152
1	-2.610599	0.539235	1.757899

$E_{(MeCN)}$ = -1019.017709
NImag = 1 (-42.0)

89. **4a**-*t* (-1014.032907) [HF/6-31+G* geometry]

6	-2.442451	-0.095090	0.870481
6	-1.158949	-0.323283	0.385232
6	-0.940203	-1.452480	-0.401777
6	-1.984860	-2.304451	-0.715941
6	-3.267074	-2.054648	-0.241603
6	-3.493294	-0.949625	0.560247
6	-0.053787	0.635026	0.752230
6	1.384750	0.032305	1.186341
6	2.276008	-0.245128	-0.038735
6	2.777571	-1.440507	-0.296790
6	3.742567	-1.767139	-1.402987
16	0.102152	2.018308	-0.574161
6	-0.087407	1.242300	-2.190935
6	-1.426247	2.971445	-0.479143
8	1.091543	-1.013386	1.912372
6	2.091540	1.150675	1.998759
1	-2.284174	2.326991	-0.601947
1	-1.455222	3.454866	0.487377
1	-1.035391	0.730503	-2.254938
1	0.722818	0.541438	-2.318571
1	-0.383190	1.237221	1.588555
1	-0.018531	2.023180	-2.936729

1	-1.404421	3.726632	-1.253840
1	3.041977	0.757490	2.340314
1	2.286703	2.068151	1.441430
1	1.498140	1.387177	2.877162
1	2.595595	0.597967	-0.643929
1	2.480610	-2.241579	0.360250
1	3.986261	-0.894155	-2.001523
1	4.670382	-2.164846	-0.998984
1	3.337901	-2.529904	-2.065198
1	0.051723	-1.680029	-0.735075
1	-1.794741	-3.178025	-1.313994
1	-4.072964	-2.725959	-0.479919
1	-4.474159	-0.758283	0.958089
1	-2.625080	0.738922	1.526790

$E_{(MeCN)}$ = -1019.020675
NImag = 0

90. **4a**-$E^{‡}$ (-1014.032155) [HF/6-31+G* geometry]

6	2.328004	-0.325139	-1.000979
6	1.063326	-0.430869	-0.428992
6	0.816119	-1.490505	0.442029
6	1.814774	-2.400619	0.743317
6	3.077548	-2.275544	0.177482
6	3.331714	-1.236488	-0.701635
6	0.025758	0.586786	-0.797998
6	-1.462434	0.185777	-1.116455
6	-2.276505	-0.205690	0.122184
6	-2.847936	-1.389828	0.253299
6	-3.748130	-1.807658	1.382922
16	0.118483	2.109932	0.625464
6	0.386354	1.337668	2.233479
6	1.716960	2.906472	0.366215
8	-1.238361	-0.774393	-1.990291
6	-2.168777	1.413022	-1.745136
1	2.515099	2.179063	0.406385
1	1.696490	3.381831	-0.604795
1	1.263129	0.708037	2.211795
1	-0.485217	0.744079	2.465251
1	0.376914	1.189287	-1.620285
1	0.496618	2.121021	2.971859
1	1.859624	3.663066	1.126609
1	-3.135241	1.078961	-2.103639
1	-2.329764	2.245277	-1.061117
1	-1.603569	1.762609	-2.604764
1	-2.474302	0.562377	0.862725
1	-2.658091	-2.109647	-0.525959
1	-3.879367	-1.014267	2.112808
1	-4.730862	-2.085217	1.009701
1	-3.351510	-2.680071	1.898227
1	-0.162894	-1.618745	0.856399
1	1.602854	-3.219483	1.407677
1	3.847110	-2.990599	0.408304
1	4.296960	-1.141834	-1.166431
1	2.526542	0.456182	-1.714249

$E_{(MeCN)}$ = -1019.020369
NImag = 1 (-245.1)

91. **4a**-PC (-1018.921039)

6	1.171399	1.813786	-1.227808
6	1.762804	0.677974	-0.652591
6	2.445545	0.811074	0.563135
6	2.521466	2.053819	1.198166
6	1.916233	3.177320	0.628433
6	1.240391	3.053831	-0.590094
6	1.664348	-0.625541	-1.371316
6	0.910711	-1.828602	-0.896743
6	0.177790	-1.841909	0.403023
6	0.730036	-2.130331	1.586508
6	-0.013187	-2.186981	2.891014
16	-3.707360	0.031792	0.220499
6	-2.909360	1.448527	1.054231
6	-3.905738	0.736746	-1.453018
8	2.349827	-1.765560	-0.832793
6	0.368032	-2.790190	-1.940356
1	-2.936708	0.995455	-1.892715
1	-4.381566	-0.028590	-2.072854
1	-1.943449	1.687497	0.598085
1	-2.742442	1.157927	2.095245
1	1.759898	-0.536135	-2.456977
1	-3.557564	2.331062	1.036250
1	-4.548682	1.623122	-1.435180
1	0.462014	-3.822688	-1.583669
1	-0.694537	-2.594728	-2.129494
1	0.916606	-2.696909	-2.883362
1	-0.892214	-1.636519	0.331638
1	1.798308	-2.345197	1.621560
1	-1.079801	-1.974467	2.758990
1	0.082672	-3.177619	3.356532
1	0.394168	-1.462153	3.609717
1	2.925333	-0.059961	0.996172
1	3.060256	2.144670	2.138254
1	1.978757	4.143338	1.123126
1	0.777244	3.924361	-1.048458
1	0.658034	1.726220	-2.183991

$E_{(MeCN)}$ = -1019.073257
NImag = 0

92. **4b**-A-*c*‡ (-1018.857565)

6	2.044587	2.379512	0.198474
16	0.607118	1.626042	-0.627088
6	-0.115028	0.531528	0.632769
6	-0.528936	3.060287	-0.743805
6	1.226964	-0.663212	1.183898
6	0.405032	-1.601976	2.093411
8	2.135873	0.031611	1.790443
6	1.630536	-1.369148	-0.105404
1	1.704214	3.149152	0.895894
1	2.508493	1.545261	0.759971
1	-0.694315	3.485686	0.249390
1	-1.471010	2.705715	-1.166617
1	-0.210799	1.113828	1.553132
1	-0.073763	3.799803	-1.409273
1	2.686474	2.802473	-0.577721
1	-0.394197	-2.139820	1.570816
6	-1.430438	0.015305	0.153958
6	-1.620537	-0.552861	-1.123406
6	-2.855155	-1.084834	-1.498956
6	-3.933761	-1.075013	-0.609056
6	-3.762839	-0.516203	0.661065
6	-2.533023	0.028697	1.032451
1	-0.793592	-0.589317	-1.828098
1	-2.971375	-1.516189	-2.490408
1	-4.892257	-1.495377	-0.901465
1	-4.591421	-0.497931	1.365008
1	-2.415736	0.461739	2.023343
1	1.104881	-2.335412	2.511798
1	-0.022774	-1.036106	2.928669
1	0.854956	-1.923501	-0.638095
6	2.890765	-1.387638	-0.557561
6	3.367809	-2.106719	-1.788717
1	3.637546	-0.855013	0.032785
1	4.126270	-2.861197	-1.535790
1	2.547327	-2.614681	-2.309540
1	3.844340	-1.415028	-2.498661

$E_{(MeCN)}$ = -1019.028465
NImag = 1 (-192.7)

93. **4b**-A-*t*‡ (-1018.843360)

6	-1.830154	2.383964	-0.474273
16	-0.338876	1.865767	0.434837
6	0.857075	3.059262	-0.300406
6	-0.032713	0.136675	-0.275089
6	1.437634	-0.148484	-0.200769
6	-1.015190	-1.276289	0.254463
6	-2.441152	-0.750282	0.432899
6	-3.443440	-1.096467	-0.383481
6	-4.885766	-0.701806	-0.225671
6	-0.467932	-1.721892	1.631402
8	-0.801999	-2.082297	-0.732619
1	-1.613930	2.420366	-1.545423
1	-2.604682	1.641615	-0.280115
1	0.867434	2.947484	-1.387430
1	1.841844	2.827038	0.106788
1	-0.374258	0.219790	-1.309864
1	0.558693	4.072261	-0.014327
1	-2.132220	3.367239	-0.105685
1	-0.516280	-0.932484	2.396379
1	-5.045438	-0.062846	0.652094
1	-5.257052	-0.165671	-1.111684
1	-5.525625	-1.588555	-0.113628
1	-2.645370	-0.143816	1.323254
1	-3.183626	-1.741225	-1.224099
1	-1.077827	-2.566520	1.973878
1	0.563801	-2.068712	1.533487
6	2.054777	-0.793587	-1.286435
6	3.404053	-1.151691	-1.233010
6	4.170066	-0.859988	-0.101626
6	3.567965	-0.223028	0.988296
6	2.215344	0.118770	0.941850
1	1.456721	-1.044217	-2.156731
1	3.855598	-1.662748	-2.079744
1	5.221492	-1.133186	-0.063961
1	4.146923	-0.005546	1.882704
1	1.758410	0.574892	1.818759

$E_{(MeCN)}$ = -1019.021260
NImag = 1 (-270.6)

94. **4b**-*c* (-1018.871181)

6	-1.816575	-2.973882	-0.152575
16	-0.977588	-1.486994	-0.802287
6	-0.060741	-0.616136	0.596818
6	0.462840	-2.440497	-1.536381
6	-1.283887	0.308949	1.004073
6	-1.248825	0.540381	2.533454
8	-2.341568	-0.476271	0.615593
6	-1.237920	1.670443	0.310906
1	-1.343198	-3.277159	0.784801
1	-2.848193	-2.686788	0.037807
1	0.966603	-3.067842	-0.793335
1	1.178052	-1.733483	-1.959399
1	0.018377	-1.391501	1.367665
1	0.061984	-3.066674	-2.339027
1	-1.735846	-3.774565	-0.893818
1	-0.353952	1.091565	2.854581

6	1.314339	-0.097488	0.277423
6	1.566450	0.760162	-0.808490
6	2.850347	1.252552	-1.046273
6	3.907692	0.908135	-0.197241
6	3.671899	0.061176	0.888017
6	2.387978	-0.441512	1.115383
1	0.749519	1.047046	-1.464521
1	3.024831	1.911521	-1.893179
1	4.905814	1.297167	-0.381401
1	4.485304	-0.213357	1.554975
1	2.213687	-1.103969	1.960849
1	-2.132113	1.118288	2.824054
1	-1.283750	-0.422056	3.058178
1	-0.419620	2.340856	0.584328
6	-2.180887	2.086314	-0.541043
6	-2.227931	3.439423	-1.195188
1	-2.988928	1.389191	-0.762662
1	-3.145292	3.979335	-0.920324
1	-1.371846	4.062634	-0.909519
1	-2.236145	3.353747	-2.291507

$E_{(MeCN)}$ = -1019.036441
NImag = 0

95. **4b**-R‡ conformer 1 (-1014.030738) [HF/6-31+G* geometry]

6	-2.335322	-0.441759	1.215932
6	-1.494921	-0.149207	0.146893
6	-2.035773	-0.135968	-1.138554
6	-3.381433	-0.387899	-1.346199
6	-4.211812	-0.677443	-0.270984
6	-3.682252	-0.710319	1.008464
6	-0.029993	0.084928	0.428843
6	1.017951	-1.214044	0.255676
6	2.301994	-0.750892	-0.452356
6	3.498675	-0.893928	0.091892
6	4.808154	-0.578343	-0.577788
16	0.481832	1.696673	-0.402489
6	-0.823702	2.882104	-0.002720
6	1.774380	2.316598	0.697493
6	0.372860	-2.262386	-0.679079
8	1.177806	-1.642475	1.476508
1	1.389282	2.378425	1.705731
1	2.599814	1.626559	0.657887
1	-1.070751	2.823360	1.048062
1	-1.693570	2.654152	-0.597511
1	0.104915	0.320420	1.471562
1	-0.458826	3.870301	-0.251039
1	2.074744	3.293000	0.341644
1	0.183994	-1.905235	-1.690732
1	-1.404323	0.054693	-1.989759
1	-3.778413	-0.372856	-2.345813
1	-5.255047	-0.882194	-0.432664
1	-4.311839	-0.946837	1.847676
1	-1.927531	-0.488672	2.209451
1	1.067541	-3.092812	-0.737247
1	-0.552598	-2.632208	-0.255857
1	2.222791	-0.398859	-1.475654
1	3.531092	-1.291714	1.092946
1	5.427316	-1.469206	-0.649572
1	4.667938	-0.186860	-1.580944
1	5.378893	0.150927	-0.005475

$E_{(MeCN)}$ = -1019.018244
NImag = 1 (-43.8)

96. **4b**-R‡ conformer 2 (-1014.025933) [HF/6-31+G* geometry]

6	-0.792700	3.130936	-0.763651
16	0.406706	2.140691	0.152416
6	-0.135725	0.369426	-0.165338
6	1.862446	2.422021	-0.879517
6	-1.391631	-0.195106	0.867846
6	-1.843202	0.927851	1.834237
8	-0.969753	-1.234127	1.504365
6	-2.516518	-0.449204	-0.144707
1	-0.835901	2.798550	-1.791786
1	-1.758643	3.024410	-0.298726
1	1.672567	2.110475	-1.896793
1	2.680895	1.852718	-0.467938
1	-0.478593	0.419477	-1.190632
1	2.093237	3.478948	-0.841240
1	-0.482181	4.165959	-0.716525
1	-2.248264	1.824887	1.365633
6	1.107666	-0.478259	-0.104269
6	1.769243	-0.718049	1.100277
6	2.929726	-1.471718	1.121635
6	3.433967	-2.024073	-0.050794
6	2.768850	-1.815575	-1.246336
6	1.615038	-1.040222	-1.268916
1	1.350688	-0.351622	2.016522
1	3.426775	-1.654044	2.057834
1	4.327812	-2.622062	-0.025448
1	3.137903	-2.253013	-2.157154
1	1.099510	-0.892297	-2.202756
1	-2.630618	0.499288	2.442383
1	-1.034166	1.207269	2.502039
1	-2.912454	0.405457	-0.684420

6	-3.028566	-1.648809	-0.353850
6	-4.148894	-1.967305	-1.304641
1	-2.608529	-2.461298	0.214892
1	-4.991998	-2.405929	-0.776078
1	-4.502902	-1.082590	-1.825624
1	-3.832620	-2.694106	-2.049623

$E_{(MeCN)}$ = -1019.013565
NImag = 1 (-38.0)

97. **4b**-*t* (-1014.033732) [HF/6-31+G* Geometry]

6	-1.751141	2.454539	-0.464530
16	-0.353187	1.807753	0.481317
6	-0.062845	0.034830	-0.250759
6	0.951712	2.850732	-0.214480
6	-1.008964	-1.157280	0.297097
6	-0.610156	-1.587119	1.724498
8	-0.792456	-2.075115	-0.613531
6	-2.456647	-0.651204	0.370760
1	-1.568952	2.325665	-1.522423
1	-2.639256	1.917353	-0.181075
1	1.036603	2.679568	-1.278489
1	1.883546	2.608568	0.269629
1	-0.376846	0.176754	-1.272453
1	0.691788	3.882168	-0.015831
1	-1.855168	3.503840	-0.222901
1	-0.665759	-0.783841	2.461963
6	1.423428	-0.230742	-0.189692
6	2.174907	-0.077022	0.972949
6	3.534181	-0.348779	0.982254
6	4.162841	-0.794778	-0.171517
6	3.420454	-0.968279	-1.329183
6	2.062244	-0.685070	-1.338278
1	1.702637	0.240336	1.886639
1	4.095844	-0.226164	1.891425
1	5.215631	-1.014422	-0.163786
1	3.893038	-1.332883	-2.223758
1	1.485112	-0.854692	-2.227835
1	-1.295856	-2.369883	2.030417
1	0.387097	-2.006536	1.725984
1	-2.724603	0.004509	1.193884
6	-3.398642	-1.069637	-0.456771
6	-4.852468	-0.689384	-0.393730
1	-3.095994	-1.763134	-1.223458
1	-5.474424	-1.569708	-0.251504
1	-5.059236	-0.001336	0.421198
1	-5.177997	-0.224133	-1.322141

$E_{(MeCN)}$ = -1019.022368
NImag = 0

98. **4b**-$E^{‡}$ (-1014.033410) [HF/6-31+G* Geometry]

6	2.148449	-0.201317	0.979111
6	1.409654	-0.293238	-0.197816
6	2.067750	-0.639373	-1.372799
6	3.433153	-0.885519	-1.374700
6	4.161678	-0.779314	-0.200315
6	3.514324	-0.435943	0.978404
6	-0.075866	-0.053971	-0.251410
16	-0.333809	1.842699	0.522917
6	1.021009	2.840942	-0.140732
6	-1.693091	2.521486	-0.456723
6	-1.040638	-1.169850	0.320992
8	-0.803350	-2.082833	-0.600848
6	-2.479384	-0.643871	0.358354
6	-3.406196	-1.046371	-0.493768
6	-4.853392	-0.637893	-0.469840
6	-0.676711	-1.615796	1.749760
1	-1.497607	2.380555	-1.511098
1	-2.600026	2.007513	-0.186813
1	1.129663	2.669420	-1.202738
1	1.931666	2.563570	0.365523
1	-0.409529	0.149940	-1.253471
1	0.799981	3.882719	0.051549
1	-1.782916	3.575466	-0.229628
1	-0.733847	-0.815180	2.488898
1	-5.067602	0.055872	0.338059
1	-5.144405	-0.168241	-1.407290
1	-5.495873	-1.505702	-0.342843
1	-2.753470	0.020867	1.171078
1	-3.097629	-1.745912	-1.252600
1	-1.381137	-2.388598	2.037758
1	0.312672	-2.053010	1.767677
1	1.501725	-0.754015	-2.278593
1	3.921938	-1.167999	-2.289970
1	5.220095	-0.970136	-0.199867
1	4.068110	-0.362723	1.897570
1	1.661495	0.045233	1.905785

$E_{(MeCN)}$ = -1019.021779
NImag = 1 (-234.4)

99. **4b**-PC (-1018.922632)

6	-1.608594	-1.492663	-0.024373
6	-1.888176	-0.150883	-0.329572
6	-3.220413	0.247576	-0.503485
6	-4.258076	-0.678072	-0.360419
6	-3.976054	-2.009188	-0.041662
6	-2.647105	-2.413728	0.124770
6	-0.753166	0.806860	-0.486222

16	2.637042	-2.015027	0.483320
6	3.223878	-3.735129	0.300840
6	3.348350	-1.286520	-1.033316
6	-0.420609	1.919858	0.461082
8	-1.053056	2.172420	-0.810135
6	0.999050	2.376159	0.568727
6	1.660282	3.043715	-0.384726
6	3.081103	3.520295	-0.273547
6	-1.271423	2.185323	1.686715
1	2.955891	-1.776007	-1.930933
1	3.058151	-0.232271	-1.050662
1	2.825446	-4.196257	-0.609063
1	2.860422	-4.294870	1.167307
1	0.097580	0.407485	-1.042262
1	4.317903	-3.779967	0.287159
1	4.441516	-1.351743	-1.027598
1	-0.804322	1.741921	2.574795
1	3.530839	3.238824	0.685336
1	3.704171	3.104844	-1.077923
1	3.138087	4.613425	-0.369173
1	1.490881	2.144871	1.515180
1	1.132578	3.273824	-1.310569
1	-1.357886	3.265651	1.853928
1	-2.274411	1.766056	1.580080
1	-3.433559	1.280720	-0.761434
1	-5.287717	-0.358393	-0.502002
1	-4.784097	-2.727849	0.070456
1	-2.418798	-3.448807	0.367411
1	-0.575163	-1.812001	0.099058

$E_{(MeCN)}$ = -1019.075619
NImag = 0

1,4- Addition (Pathway 5)

100. **5a**-A-*c*‡ (-1018.862078)

6	0.521552	2.832177	-1.132743
1	1.503103	2.757443	-0.658247
1	0.613282	2.686070	-2.211278
16	-0.597149	1.510173	-0.492549
6	-0.598440	1.999030	1.261522
1	0.420140	2.070026	1.647713
1	-1.214700	1.258141	1.775158
6	0.229545	-0.050145	-0.646734
1	0.060772	-0.329914	-1.688436
6	-1.150208	-1.572994	0.126250
6	-0.350262	-2.780571	-0.303298
1	-0.733628	-3.667144	0.221114
1	-0.453679	-2.968775	-1.378913
1	0.713426	-2.690280	-0.065667
6	-2.447579	-1.390482	-0.365073
1	-2.761823	-1.936832	-1.252813
6	-3.369428	-0.492043	0.252024
6	-4.806733	-0.457832	-0.256678
1	-4.981685	-1.141118	-1.094663
1	-5.484340	-0.722749	0.564195
1	-5.062678	0.562993	-0.566517
8	-3.060206	0.276747	1.197549
1	-1.098291	2.970373	1.308554
1	0.064539	3.805442	-0.929354
6	1.638659	-0.174610	-0.219841
6	2.645587	-0.469297	-1.167079
6	3.971109	-0.674440	-0.783960
6	4.339786	-0.581448	0.562362
6	3.358420	-0.304046	1.518629
6	2.028316	-0.115291	1.137608
1	2.375751	-0.537374	-2.219149
1	4.719854	-0.900071	-1.539786
1	5.372728	-0.735829	0.862679
1	3.624455	-0.255013	2.572010
1	1.276554	0.034665	1.906460
1	-0.979686	-1.244847	1.149401

$E_{(MeCN)}$ = -1019.028953
NImag = 1 (-241.7)

101. **5a**-A-*t*‡ (-1018.851413)

6	-2.107594	-2.154393	-1.604358
1	-2.856113	-1.512174	-1.136267
1	-1.855455	-1.774501	-2.596395
16	-0.545950	-2.148203	-0.623264
6	-1.176967	-2.911962	0.914167
1	-2.027224	-2.365628	1.324958
1	-0.354000	-2.931082	1.629762
6	0.012756	-0.483049	-0.265845
1	0.775457	-0.357909	-1.034919
6	1.373960	-0.389019	1.211872
6	0.605203	-0.166172	2.498344
1	1.281686	-0.304141	3.352301
1	0.207260	0.852920	2.551670
1	-0.234903	-0.857339	2.627555
6	2.309992	0.596002	0.815903
1	2.260381	1.590953	1.253123
6	3.212097	0.332910	-0.253290
6	4.276753	1.372545	-0.593110
1	4.203660	2.275695	0.023331
1	5.270140	0.929088	-0.450396
1	4.199551	1.650816	-1.651460
8	3.158851	-0.717157	-0.945091
1	-1.466509	-3.936874	0.666578

1	-2.462718	-3.186391	-1.679781
6	-0.970396	0.619719	-0.207395
6	-0.650458	1.826693	-0.866261
6	-1.481899	2.944525	-0.776003
6	-2.669649	2.887471	-0.042020
6	-3.003989	1.701180	0.619437
6	-2.161508	0.591146	0.548753
1	0.262746	1.879607	-1.452104
1	-1.202989	3.860597	-1.291121
1	-3.322443	3.754070	0.019994

$E_{(MeCN)}$ = -1019.024734
NImag = 1 (-349.6)

102. **5a**-*c* (-1018.889771)

6	0.156607	2.354667	-1.588650
1	1.226564	2.290528	-1.372764
1	-0.049424	1.986504	-2.597360
16	-0.876811	1.366795	-0.403334
6	-0.250447	2.181910	1.106808
1	0.839932	2.150621	1.149349
1	-0.718158	1.669301	1.945142
6	0.027571	-0.298567	-0.645789
1	0.019226	-0.322963	-1.742413
6	-0.839216	-1.494018	-0.147968
6	-0.284664	-2.778557	-0.790870
1	-0.834157	-3.642834	-0.401874
1	-0.420840	-2.763216	-1.880847
1	0.780312	-2.930008	-0.580784
6	-2.314607	-1.329862	-0.405579
1	-2.816524	-2.013340	-1.085491
6	-3.006142	-0.448235	0.388104
6	-4.517800	-0.338540	0.354255
1	-4.971071	-1.044325	-0.351494
1	-4.923502	-0.533196	1.355664
1	-4.818447	0.681494	0.080548
8	-2.365538	0.359741	1.187945
1	-0.600560	3.217046	1.057326
1	-0.177441	3.393953	-1.518751
6	1.454740	-0.271034	-0.154698
6	2.514086	-0.172023	-1.072201
6	3.844232	-0.201564	-0.645304
6	4.138745	-0.327380	0.714457
6	3.095062	-0.429058	1.639618
6	1.766679	-0.402300	1.210524
1	2.295674	-0.092085	-2.135040
1	4.646954	-0.131988	-1.374991
1	5.172038	-0.352702	1.050582
1	3.314560	-0.534414	2.699019
1	0.966089	-0.491552	1.938797
1	-0.687011	-1.556101	0.938908

$E_{(MeCN)}$ = -1019.059132
NImag = 0

103. **5a**-$R^{‡}$ (-1018.878868)

16	-0.295451	1.968405	0.243128
6	-0.022578	0.080930	0.099143
6	-0.754514	-0.729078	1.244087
6	-1.835598	-1.578318	0.612135
6	-2.710725	-1.128480	-0.358495
8	-2.716453	0.074978	-0.852164
6	-3.743211	-2.091504	-0.931370
6	1.462400	-0.118077	-0.105722
6	1.875754	-0.924248	-1.179230
6	3.230549	-1.192373	-1.394127
6	4.196622	-0.643778	-0.547920
6	3.798872	0.169427	0.518350
6	2.445112	0.426525	0.738693
6	-1.953874	2.230307	0.964821
6	-0.663471	2.327572	-1.506372
1	-1.882966	2.079104	2.042934
1	-2.629242	1.513114	0.472508
1	-2.209818	3.273903	0.756485
1	-1.504993	1.685047	-1.792117
1	-0.899530	3.390644	-1.595398
1	0.236992	2.099025	-2.081292
1	1.126752	-1.354581	-1.839570
1	3.528140	-1.825020	-2.226406
1	2.154289	1.057790	1.574878
1	4.543657	0.602096	1.181517
1	5.251221	-0.844529	-0.717715
1	-0.562968	-0.129527	-0.821930
1	-1.178810	0.003940	1.951751
6	0.200681	-1.595918	2.083133
1	0.964622	-1.006891	2.602543
1	0.706765	-2.347242	1.466807
1	-0.387173	-2.126206	2.841016
1	-1.909107	-2.604902	0.962486
1	-3.690120	-3.091032	-0.484094
1	-4.751197	-1.686178	-0.772854
1	-3.603794	-2.180786	-2.017044

$E_{(MeCN)}$ = -1019.048135
NImag = 1 (-37.8)

104. **5a**-*t* (-1014.075851) [HF/6-31+G* Geometry]

6	-1.857143	2.610931	0.053850
1	-2.402196	1.817191	-0.446297
1	-2.219221	2.742181	1.061868

16	-0.100978	2.153571	0.148709
6	0.436472	2.535633	-1.530707
1	-0.213391	2.039917	-2.238781
1	1.453386	2.192348	-1.646128
6	-0.132879	0.273393	0.107691
1	-0.694104	0.100811	-0.793805
6	-1.006823	-0.298486	1.272336
6	-0.240550	-0.596290	2.559864
1	-0.946133	-0.930164	3.313210
1	0.492192	-1.383268	2.421098
1	0.273351	0.277282	2.955970
6	-1.733004	-1.500442	0.724745
1	-1.562693	-2.462446	1.174098
6	-2.633347	-1.321356	-0.293317
6	-3.412673	-2.507192	-0.828518
1	-3.168055	-3.435925	-0.323319
1	-4.475934	-2.314643	-0.717014
1	-3.218048	-2.619944	-1.891651
8	-2.853581	-0.199607	-0.848153
1	0.395390	3.608065	-1.663749
1	-1.909749	3.554610	-0.472800
6	1.285757	-0.229504	-0.053212
6	1.528343	-1.191699	-1.029610
6	2.801800	-1.712762	-1.212442
6	3.855882	-1.267311	-0.430786
6	3.627163	-0.303851	0.541434
6	2.351978	0.205433	0.732097
1	0.713675	-1.546620	-1.633977
1	2.966174	-2.462901	-1.965157
1	4.844093	-1.666307	-0.574547
1	4.437114	0.045347	1.156849
1	2.196238	0.939037	1.502777
1	-1.743654	0.466172	1.506679

$E_{(MeCN)}$ = -1019.050220
NImag = 0

105. **5a**-$E^{‡}$ (-1014.070517) [HF/6-31+G* Geometry]

16	0.031692	2.330637	0.125067
6	-1.689367	2.828365	-0.158007
6	0.723526	2.561581	-1.526493
6	-0.206205	0.156258	0.146948
6	-1.137798	-0.203805	1.284697
6	-1.695161	-1.479331	0.708774
6	-2.598819	-1.381980	-0.337517
8	-2.917880	-0.292346	-0.874071
6	-3.233996	-2.643573	-0.891271
6	-0.533871	-0.352039	2.675788
1	-2.212694	2.064341	-0.718608
1	-1.692815	3.777063	-0.678720
1	-2.158407	2.953430	0.806839
1	0.700249	3.613465	-1.778488
1	1.747650	2.218298	-1.511872
1	0.156347	1.995133	-2.253512
1	-0.755312	0.170830	-0.773494
1	-1.926661	0.539088	1.318586
1	-1.402897	-2.422527	1.132923
1	-2.886755	-3.544109	-0.396021
1	-4.312013	-2.573923	-0.781066
1	-3.024458	-2.718163	-1.954524
1	-0.084560	0.571109	3.035291
1	0.215812	-1.134312	2.713829
1	-1.325646	-0.623297	3.365437
6	1.189749	-0.366697	0.005530
6	1.494612	-1.128233	-1.120197
6	2.769640	-1.641576	-1.305892
6	3.763185	-1.383271	-0.374259
6	3.474818	-0.613358	0.744270
6	2.197008	-0.112354	0.934645
1	0.723850	-1.339220	-1.839202
1	2.982942	-2.240185	-2.173193
1	4.753781	-1.776667	-0.517192
1	4.241594	-0.406044	1.469093
1	1.992042	0.484347	1.803300

$E_{(MeCN)}$ = -1019.048606
NImag = 1 (-359.7)

106. **5a**-PC (-1018.954279)

6	3.678130	-1.064633	1.276462
1	3.351172	-0.035907	1.099100
1	3.424067	-1.355813	2.299964
16	2.807534	-2.216544	0.154565
6	3.306867	-1.498811	-1.450848
1	3.007107	-0.448443	-1.513569
1	2.797615	-2.068327	-2.233801
6	-0.464004	0.435633	0.278135
1	0.439886	-0.142463	0.094151
6	-0.316908	1.409127	1.419411
6	-1.451178	1.784178	2.348533
1	-1.288958	2.781687	2.775407
1	-2.420925	1.785200	1.841381
1	-1.515981	1.069814	3.178728
6	-0.281519	1.929979	-0.014376
1	-1.157992	2.479750	-0.348350
6	1.016318	2.374103	-0.596260
6	0.962523	3.514795	-1.594471

1	0.324416	3.243351	-2.445857
1	0.514985	4.404229	-1.131513
1	1.967423	3.753015	-1.950024
8	2.079132	1.846383	-0.287003
1	4.388495	-1.584316	-1.600194
1	4.763407	-1.139301	1.149513
6	-1.717880	-0.318008	-0.037291
6	-2.917216	0.276953	-0.458562
6	-4.050681	-0.497890	-0.722439
6	-4.006869	-1.886122	-0.575760
6	-2.815647	-2.493579	-0.167322
6	-1.685674	-1.717813	0.096000
1	-2.975517	1.352916	-0.597932
1	-4.967276	-0.012629	-1.049273
1	-4.887792	-2.488009	-0.783745
1	-2.763030	-3.574085	-0.057956
1	-0.758987	-2.197371	0.403303
1	0.666730	1.382879	1.886386

$E_{(MeCN)}$ = -1019.109599
NImag = 0

107. **5b**-A-*c*‡ (-1018.852565)

6	0.623943	2.627872	-1.484593
1	1.638674	2.518528	-1.095944
1	0.569165	2.232234	-2.500984
16	-0.561228	1.661871	-0.476943
6	-0.419557	2.554347	1.112911
1	0.614744	2.640532	1.446840
1	-1.014961	2.001004	1.838889
6	0.042759	0.006127	-0.301081
1	-0.483879	-0.515988	-1.104810
6	-1.141123	-0.973554	1.066741
6	-0.512163	-0.800724	2.432005
1	-0.884300	0.089250	2.954375
1	-0.774259	-1.666879	3.055045
1	0.580841	-0.752384	2.385716
1	-0.823704	-1.886319	0.562565
6	-2.501156	-0.638447	0.868813
1	-3.024303	-0.034632	1.609393
6	-3.159644	-1.004050	-0.340231
6	-4.652178	-0.716057	-0.482568
1	-5.078800	-0.218592	0.396088
1	-4.826597	-0.093227	-1.368819
1	-5.185492	-1.660703	-0.645135
8	-2.562095	-1.543326	-1.306893
1	-0.855556	3.545451	0.960824
1	0.310479	3.675860	-1.477048
6	1.479973	-0.296509	-0.233266
6	1.942021	-1.432790	-0.939767
6	3.269158	-1.850808	-0.857685
6	4.192326	-1.140891	-0.082000
6	3.758029	-0.015614	0.624347
6	2.424504	0.392749	0.560997
1	1.240338	-1.986491	-1.559350
1	3.586500	-2.730337	-1.412931
1	5.229006	-1.461322	-0.025104
1	4.457729	0.542742	1.242205
1	2.119416	1.248038	1.156679

$E_{(MeCN)}$ = -1019.024693
NImag = 1 (-334.5)

108. **5b**-A-*t*‡ (-1018.861635)

6	-2.228675	2.573480	-0.849814
1	-2.531385	1.654110	-1.356714
1	-2.921490	2.805096	-0.038257
16	-0.556686	2.339870	-0.108267
6	0.392174	2.087351	-1.648651
1	-0.185861	1.473697	-2.343110
1	1.342177	1.587456	-1.400710
6	-0.526036	0.842367	0.848573
1	-0.924227	1.161187	1.813367
6	1.492546	0.462672	1.422203
6	1.284288	0.509999	2.924127
1	0.684156	-0.339127	3.273601
1	2.258930	0.449853	3.426740
1	0.800420	1.436228	3.254764
1	1.896509	1.381242	0.998136
6	1.995832	-0.715420	0.844257
1	1.865729	-1.658220	1.371667
6	2.665018	-0.726988	-0.411242
6	3.318022	-2.026283	-0.871450
1	3.148092	-2.859441	-0.181272
1	2.937268	-2.298604	-1.863600
1	4.398413	-1.867364	-0.976708
8	2.763801	0.275924	-1.169772
1	0.565719	3.080371	-2.073047
1	-2.182530	3.410262	-1.553224
6	-1.189292	-0.368729	0.328123
6	-2.227229	-0.970481	1.071504
6	-2.826838	-2.157707	0.652051
6	-2.410051	-2.775361	-0.532680
6	-1.373386	-2.203328	-1.273526
6	-0.756108	-1.025024	-0.843383
1	-2.567084	-0.493418	1.989024
1	-3.626500	-2.595860	1.244650
1	-2.880583	-3.696664	-0.866304

1	-1.023706	-2.686791	-2.182637
1	0.080932	-0.628624	-1.406460

$E_{(MeCN)}$ = -1019.029468
NImag = 1 (-262.5)

109. **5b**-*c* (-1018.878469)

6	0.269958	2.593433	-0.033839
1	1.300172	2.399946	0.273801
1	0.207421	2.673107	-1.121622
16	-0.894486	1.248371	0.466698
6	-0.485171	1.243093	2.247651
1	0.586642	1.129607	2.420233
1	-1.050060	0.430255	2.704390
6	-0.028411	-0.242437	-0.371885
1	-0.370449	0.000055	-1.382900
6	-0.862974	-1.491089	0.031847
6	-0.334236	-2.330419	1.204514
1	-0.345862	-1.782318	2.155435
1	-0.990327	-3.199392	1.330064
1	0.680144	-2.704014	1.031053
1	-0.781602	-2.126539	-0.870771
6	-2.303488	-1.080837	0.253744
1	-2.845647	-1.604445	1.038991
6	-3.028481	-0.389522	-0.728343
6	-4.529982	-0.193395	-0.535953
1	-4.914296	-0.672646	0.372043
1	-4.760335	0.879549	-0.498724
1	-5.060843	-0.602971	-1.404470
8	-2.493839	0.156165	-1.749248
1	-0.826631	2.199979	2.654067
1	-0.100361	3.519728	0.413885
6	1.476918	-0.243184	-0.322812
6	2.173340	-0.025880	-1.526064
6	3.569080	-0.041118	-1.572113
6	4.304380	-0.260332	-0.404966
6	3.631249	-0.473515	0.801374
6	2.234987	-0.471084	0.841004
1	1.609138	0.145885	-2.439857
1	4.078989	0.119518	-2.518520
1	5.390807	-0.270175	-0.434477
1	4.193376	-0.653659	1.714299
1	1.739196	-0.667011	1.784935

$E_{(MeCN)}$ = -1019.052119
NImag = 0

110. **5b**-$R^{‡}$ (-1018.861649)

6	3.059760	-1.784326	-0.503843
1	3.505222	-1.676719	0.487978
1	2.456356	-2.691858	-0.553901
16	1.962345	-0.377594	-0.881689
6	3.116390	1.008135	-0.616550
1	3.561827	0.954980	0.380384
1	2.542540	1.930236	-0.722928
6	0.735947	-0.270593	0.630645
1	1.413909	-0.163939	1.488274
6	-0.048074	-1.643666	0.705658
6	0.526839	-2.468546	1.874257
1	0.263606	-2.010803	2.837293
1	0.095758	-3.474225	1.859172
1	1.622503	-2.567703	1.845326
1	0.137982	-2.170814	-0.244809
6	-1.532305	-1.505271	0.793551
1	-2.004189	-1.485534	1.772940
6	-2.274494	-1.546522	-0.381563
6	-3.797904	-1.584384	-0.300836
1	-4.170053	-1.575667	0.730929
1	-4.220255	-0.724298	-0.837317
1	-4.167528	-2.487302	-0.803880
8	-1.746453	-1.544009	-1.551178
6	0.021805	1.037207	0.404584
1	3.891593	0.962885	-1.386693
1	3.835712	-1.818035	-1.273110
6	-0.810339	1.244476	-0.710192
6	-1.399420	2.493734	-0.910365
6	-1.177468	3.542977	-0.010502
6	-0.358972	3.339719	1.102710
6	0.245387	2.094655	1.301206
1	-1.025297	0.411734	-1.383412
1	-2.049749	2.641725	-1.768743
1	-1.645878	4.510646	-0.172995
1	-0.188640	4.143915	1.814139
1	0.875782	1.938791	2.175245

$E_{(MeCN)}$ = -1019.043960
NImag = 1 (-43.7)

111. **5b**-*t* (-1018.874913)

6	2.258559	-2.347816	-0.711366
1	2.645784	-1.364505	-0.987638
1	2.731834	-2.697527	0.209247
16	0.461309	-2.256620	-0.431770
6	-0.159374	-1.635546	-2.022035
1	0.594180	-0.993902	-2.483718
1	-1.089352	-1.051347	-1.802301
6	0.249348	-0.834353	0.817644
1	0.762273	-1.294642	1.671598
6	-1.320860	-0.775578	1.152689
6	-1.487143	-1.249818	2.609867

1	-1.033722	-0.533288	3.307922
1	-2.551436	-1.322885	2.854231
1	-1.028841	-2.233403	2.786773
1	-1.802183	-1.522539	0.501034
6	-2.016926	0.526011	0.911925
1	-2.175048	1.182814	1.764265
6	-2.556251	0.832143	-0.321717
6	-3.397151	2.091553	-0.485462
1	-3.511639	2.651672	0.450041
1	-2.943932	2.749645	-1.239317
1	-4.392484	1.818967	-0.859386
8	-2.377014	0.120440	-1.388376
1	-0.365513	-2.510872	-2.643277
1	2.432474	-3.072664	-1.510909
6	1.015495	0.400660	0.431240
6	2.172892	0.724112	1.159582
6	2.923333	1.863616	0.854866
6	2.526986	2.691746	-0.197381
6	1.375923	2.380011	-0.928461
6	0.615162	1.250806	-0.616587
1	2.481772	0.088221	1.987824
1	3.809853	2.100172	1.437702
1	3.105763	3.579077	-0.441671
1	1.054109	3.029476	-1.738533
1	-0.288691	1.034648	-1.177397

$E_{(MeCN)}$ = -1019.050258
NImag = 0

112. **5b**-$E^{‡}$ (-1018.871077)

16	-1.109264	-2.162470	0.429671
6	-0.630065	-1.490369	2.061100
6	-2.890068	-1.784229	0.399123
6	-0.157810	-0.736312	-0.854864
6	1.325328	-1.171721	-0.748130
6	1.601368	-2.260119	-1.801780
6	2.241444	0.004598	-0.857761
6	2.719813	0.572551	0.319841
8	2.314684	0.209322	1.484054
6	3.762111	1.680874	0.254180
1	0.423949	-1.186928	2.013430
1	-0.775075	-2.276670	2.805972
1	-1.245236	-0.618560	2.292424
1	-3.370009	-2.267585	1.254826
1	-3.044958	-0.702469	0.432170
1	-3.302710	-2.193422	-0.526236
1	-0.588578	-1.091545	-1.798286
1	0.891488	-3.097277	-1.739466
1	1.545388	-1.844420	-2.816686
1	2.609890	-2.660857	-1.661323
1	1.506845	-1.595917	0.249027
1	2.578713	0.332711	-1.837412
1	3.366238	2.591609	0.723149
1	4.648349	1.384420	0.829242
1	4.066674	1.916764	-0.772279
6	-0.736961	0.599022	-0.534365
6	-0.368594	1.381640	0.579877
6	-1.011503	2.593464	0.826821
6	-2.032196	3.053122	-0.015774
6	-2.404398	2.290805	-1.124435
6	-1.763944	1.074900	-1.375775
1	0.450270	1.055098	1.219326
1	-0.702670	3.191397	1.680729
1	-2.524798	4.000817	0.187045
1	-3.184058	2.640641	-1.796417
1	-2.046115	0.497776	-2.254764

$E_{(MeCN)}$ = -1019.045301
NImag = 1 (-163.8)

113. **5b**-PC (-1018.950324)

6	5.495410	-0.983826	0.020439
1	5.685678	-0.781853	1.079967
1	5.769637	-2.020750	-0.194055
16	3.724021	-0.798743	-0.383875
6	3.493771	0.964373	0.033325
1	3.702002	1.151892	1.091961
1	2.447851	1.211203	-0.168029
6	-0.958682	-0.619939	0.859834
1	-0.662342	-0.759902	1.899191
6	-0.751343	-1.823515	-0.003076
6	0.045150	-3.009264	0.502697
1	-0.132406	-3.180286	1.571980
1	-0.230957	-3.925049	-0.034557
1	1.119421	-2.839706	0.364193
1	-0.646221	-1.619344	-1.067304
6	-2.153545	-1.566842	0.501717
1	-2.499598	-2.159318	1.347419
6	-3.228643	-1.125244	-0.433436
6	-4.646024	-1.160355	0.109845
1	-4.920036	-2.184034	0.397695
1	-4.722231	-0.541729	1.013679
1	-5.344979	-0.795014	-0.645763
8	-2.993232	-0.749059	-1.574203
6	-0.846522	0.807553	0.433284
1	4.133090	1.602300	-0.586102
1	6.113994	-0.322623	-0.595735
6	-0.726322	1.218882	-0.904671
6	-0.603631	2.573280	-1.225889
6	-0.593565	3.544893	-0.221596

6	-0.707181	3.149629	1.114429
6	-0.831833	1.796495	1.433635
1	-0.746405	0.484939	-1.701953
1	-0.517790	2.867157	-2.269118
1	-0.497487	4.597315	-0.476518
1	-0.697006	3.892646	1.908307
1	-0.914927	1.497784	2.477145

$E_{(MeCN)}$ = -1019.107030
NImag = 0

Reactant Geometries

114. Dimethylsulfonium benzylide (*In* conformer) (-748.307813)

6	-2.454508	0.664314	-1.388215
1	-1.746036	1.493816	-1.357196
1	-2.327522	0.098926	-2.313497
1	-3.481420	1.034507	-1.310338
16	-2.163702	-0.543530	-0.000044
6	-2.454362	0.663944	1.388454
1	-1.746270	1.493757	1.357205
1	-3.481474	1.033698	1.311163
1	-2.326652	0.098467	2.313582
6	-0.612839	-1.174071	-0.000161
1	-0.645111	-2.257651	-0.000308
6	0.666722	-0.499403	-0.000080
6	1.845564	-1.290323	-0.000057
6	3.113572	-0.718219	0.000015
6	3.273252	0.673837	0.000066
6	2.128141	1.474135	0.000033
6	0.853711	0.904484	-0.000044
1	1.747876	-2.374126	-0.000092
1	3.988282	-1.365383	0.000032
1	4.263843	1.120236	0.000122
1	2.222857	2.558251	0.000058
1	-0.004657	1.569795	-0.000096

$E_{(MeCN)}$ = -748.411684
NImag = 0

115. Dimethylsulfonium benzylide (*In* conformer) (-745.220436) [HF/6-31+G* Geometry]

6	2.443430	0.637318	1.379798
1	1.747805	1.462898	1.372804
1	2.319285	0.065715	2.288320
1	3.459759	1.006564	1.313938
16	2.155219	-0.511423	-0.000013
6	2.443520	0.637474	-1.379677
1	1.748056	1.463188	-1.372508
1	3.459923	1.006518	-1.313841
1	2.319197	0.066027	-2.288273
6	0.619577	-1.158259	-0.000091
1	0.654455	-2.229295	-0.000131
6	-0.664018	-0.486192	-0.000047
6	-1.828756	-1.281096	-0.000023
6	-3.089899	-0.723194	0.000014
6	-3.263645	0.658605	0.000032
6	-2.134246	1.457509	0.000008
6	-0.861055	0.902748	-0.000034
1	-1.726140	-2.352430	-0.000033
1	-3.949883	-1.371001	0.000031
1	-4.247697	1.091636	0.000063
1	-2.235444	2.529652	0.000017
1	-0.022272	1.573824	-0.000063

$E_{(MeCN)}$ = -748.410004
NImag = 0

116. Dimethylsulfonium benzylide (*Out* conformer) (-748.306682)

6	3.110068	0.200417	-1.323568
1	4.016584	-0.410605	-1.267000
1	2.624151	0.072765	-2.292576
1	3.348133	1.255883	-1.161646
16	1.896516	-0.360935	-0.045248
6	3.021526	-0.098682	1.416190
1	2.450482	-0.390629	2.299670
1	3.913818	-0.725475	1.315949
1	3.297526	0.958021	1.481175
6	0.621913	0.721245	-0.008759
1	0.864144	1.776836	0.085656
6	-0.769544	0.302518	-0.006477
6	-1.217448	-1.038782	-0.089355
6	-2.575208	-1.353358	-0.088811
6	-3.549773	-0.352251	-0.005728
6	-3.128150	0.979075	0.077124
6	-1.771965	1.300249	0.077952
1	-0.492845	-1.847221	-0.156347
1	-2.874645	-2.397652	-0.154310
1	-4.607004	-0.603266	-0.005239
1	-3.862396	1.779564	0.143283
1	-1.470725	2.344143	0.143943

$E_{(MeCN)}$ = -748.411181
NImag = 0

117. Dimethylsulfonium benzylide (*Out* conformer (-745.220044) [HF/6-31+G* Geometry]

6	3.116729	0.127247	-1.279329
1	4.009054	-0.477322	-1.171538
1	2.664009	-0.045159	-2.244663

1	3.359377	1.176790	-1.174135
16	1.900230	-0.350094	-0.029702
6	2.912781	-0.042368	1.448070
1	2.300381	-0.283524	2.305235
1	3.792318	-0.675292	1.432358
1	3.200553	1.000569	1.489192
6	0.628739	0.726872	-0.110608
1	0.870018	1.771093	-0.021631
6	-0.760434	0.303761	-0.054537
6	-1.202445	-1.029633	-0.100470
6	-2.550728	-1.344525	-0.058978
6	-3.520473	-0.356198	0.026913
6	-3.101003	0.967532	0.071472
6	-1.757587	1.291976	0.034768
1	-0.489910	-1.832347	-0.174380
1	-2.843964	-2.380123	-0.097058
1	-4.565501	-0.607325	0.057476
1	-3.828488	1.758750	0.138163
1	-1.465006	2.327409	0.072412

$E_{(MeCN)}$ = -748.409684
NImag = 0

118. Dienal conformer 1 (2*E*,4*E*-*trans*,*trans*) (-500.405197)

8	5.769249	0.367418	-0.000069
6	4.713150	-0.249349	0.000035
6	3.389950	0.369360	-0.000081
6	2.260163	-0.382927	0.000027
6	0.915776	0.137242	-0.000104
6	-0.179953	-0.662757	0.000063
1	4.716408	-1.362243	0.000183
1	3.354511	1.457443	-0.000263
1	2.364164	-1.470287	0.000211
1	0.810513	1.220912	-0.000279
1	-0.013346	-1.740975	0.000293
6	-1.584980	-0.258694	0.000044
6	-2.576321	-1.260586	0.000037
6	-3.932785	-0.935349	-0.000002
6	-4.329557	0.404302	-0.000009
6	-3.358038	1.413443	0.000007
6	-2.004292	1.088533	0.000041
1	-2.273147	-2.305437	0.000045
1	-4.678135	-1.726338	-0.000015
1	-5.385095	0.662899	-0.000032
1	-3.659781	2.457681	0.000001
1	-1.268767	1.887693	0.000058

$E_{(MeCN)}$ = -500.520618
NImag = 0

119. Dienal conformer 2 (2*E*,4*E*-*cis*,*trans*) (-500.402672)

6	-0.073055	-0.520221	-0.000003
6	0.957258	0.364113	0.000207
6	2.334409	-0.054208	0.000073
6	3.402197	0.785050	0.000230
6	4.785026	0.291552	0.000134
8	5.113170	-0.888248	-0.000363
1	0.180153	-1.581133	-0.000264
1	0.766540	1.436429	0.000404
1	2.536963	-1.125607	-0.000146
1	3.264183	1.865693	0.000444
1	5.567611	1.079088	0.000020
6	-1.505110	-0.228432	-0.000035
6	-2.414439	-1.305546	0.000095
6	-3.792198	-1.087889	0.000121
6	-4.293662	0.216294	-0.000021
6	-3.404811	1.299010	-0.000171
6	-2.029772	1.081510	-0.000191
1	-2.029807	-2.323140	0.000206
1	-4.472926	-1.935168	0.000240
1	-5.366366	0.390536	-0.000013
1	-3.787898	2.316248	-0.000291
1	-1.358874	1.935652	-0.000326

$E_{(MeCN)}$ = -500.517992
NImag = 0

120. Dienal conformer 3 (2*E*,4*E*-*trans*,*cis*) (-500.399420)

6	0.025727	0.082583	0.000164
6	0.854884	-0.990254	0.000161
6	2.306804	-0.941432	0.000248
6	3.118018	0.146445	-0.000154
6	4.570470	-0.007311	0.000029
8	5.367508	0.920507	-0.000285
1	0.471544	1.076830	0.000298
1	0.427621	-1.990670	0.000138
1	2.798405	-1.915939	0.000649
1	2.741660	1.166950	-0.000673
1	4.935843	-1.058387	0.000501
6	-1.436495	0.076110	0.000066
6	-2.114512	1.312056	0.000181
6	-3.508014	1.372626	0.000092
6	-4.258190	0.194211	-0.000122
6	-3.601689	-1.043405	-0.000239
6	-2.211152	-1.103552	-0.000144
1	-1.535638	2.233106	0.000346
1	-4.006687	2.338295	0.000200
1	-5.344133	0.236105	-0.000217

1	-4.179220	-1.964260	-0.000417
1	-1.724568	-2.074546	-0.000237

$E_{(MeCN)}$ = -500.514703
NImag = 0

121. Dienal conformer 4 (2*E*,4*E*-*cis*,*cis*)
(-500.396307)

6	0.016191	0.246537	-0.009617
6	0.940487	-0.746281	-0.031316
6	2.381112	-0.568322	-0.031345
6	3.090607	0.584108	0.075990
6	4.559885	0.587115	0.052477
8	5.269203	-0.403167	-0.069318
1	0.369448	1.277443	-0.004697
1	0.605334	-1.780880	-0.060362
1	2.971641	-1.478954	-0.126988
1	2.608154	1.553054	0.190974
1	5.029373	1.587873	0.157829
6	-1.439109	0.108497	-0.002859
6	-2.104006	-1.135735	0.039699
6	-3.494313	-1.201474	0.041502
6	-4.260364	-0.029189	0.003258
6	-3.619908	1.211757	-0.036377
6	-2.226732	1.277316	-0.038367
1	-1.531160	-2.057639	0.074362
1	-3.985990	-2.170300	0.075144
1	-5.345642	-0.085749	0.005631
1	-4.204008	2.127862	-0.065563
1	-1.733869	2.246659	-0.070058

$E_{(MeCN)}$ = -500.511638
NImag = 0

122. Dienal conformer 5 (2*Z*,4*E*-*trans*,*trans*)
(-500.400370)

6	-0.154447	-0.984940	-0.000014
6	1.061080	-0.382404	-0.000044
1	-0.172453	-2.075951	0.000019
1	1.128294	0.702017	-0.000057
6	2.287452	-1.146919	-0.000030
6	3.567893	-0.684077	-0.000009
1	2.154531	-2.229799	-0.000046
1	4.393122	-1.392812	-0.000019
6	3.967379	0.722861	0.000014
8	5.134501	1.092137	-0.000092
1	3.157248	1.480149	-0.000002
6	-1.471665	-0.349965	0.000007
6	-2.616938	-1.171460	0.000099
6	-3.899680	-0.623407	0.000122
6	-4.066632	0.763763	0.000058
6	-2.939768	1.595798	-0.000034
6	-1.659643	1.048362	-0.000059
1	-2.493236	-2.252346	0.000155
1	-4.767005	-1.278430	0.000192
1	-5.063998	1.195384	0.000072
1	-3.062000	2.675854	-0.000097
1	-0.800695	1.713172	-0.000137

$E_{(MeCN)}$ = -500.515222
NImag = 0

123. Dienal conformer 6 (2*Z*,4*E*-*cis*,*trans*)
(-500.401187)

6	0.002060	-1.049891	0.000083
6	1.216964	-0.441348	0.000032
1	-0.018632	-2.141366	0.000135
1	1.313179	0.638872	-0.000045
6	2.437357	-1.206659	0.000059
6	3.714161	-0.726462	0.000026
1	2.317543	-2.291631	0.000118
1	4.535313	-1.440951	0.000057
6	4.119250	0.682243	-0.000037
8	3.374577	1.657214	-0.000152
1	5.218747	0.840118	-0.000097
6	-1.311174	-0.410133	0.000048
6	-2.462593	-1.223339	-0.000086
6	-3.740764	-0.665192	-0.000136
6	-3.895727	0.723462	-0.000047
6	-2.762335	1.546819	0.000096
6	-1.486473	0.990303	0.000143
1	-2.347026	-2.305181	-0.000153
1	-4.613697	-1.312786	-0.000243
1	-4.889664	1.163129	-0.000082
1	-2.876207	2.627762	0.000175
1	-0.620540	1.645502	0.000264

$E_{(MeCN)}$ = -500.514459
NImag = 0

124. Dienal conformer 7 (2*Z*,4*E*-*trans*,*cis*)
(-500.393498)

6	0.289334	-0.190601	-0.386616
6	1.032396	-1.313513	-0.235062
1	0.787464	0.703016	-0.760339
1	0.535052	-2.251601	0.009642
6	2.464586	-1.416254	-0.475330
6	3.432458	-0.492087	-0.239694

1	2.788341	-2.367982	-0.900122
1	4.452591	-0.694743	-0.560139
6	3.261077	0.757710	0.508492
8	4.121486	1.626399	0.574252
1	2.314407	0.872352	1.071193
6	-1.151380	-0.043928	-0.163611
6	-1.781140	1.144535	-0.582790
6	-3.150484	1.339174	-0.400346
6	-3.921744	0.347983	0.211551
6	-3.310521	-0.836264	0.642149
6	-1.943498	-1.029643	0.460444
1	-1.185516	1.920317	-1.058994
1	-3.613566	2.264107	-0.733973
1	-4.988271	0.496528	0.358343
1	-3.902556	-1.607648	1.127985
1	-1.486340	-1.948192	0.817269

$E_{(MeCN)}$ = -500.507435
NImag = 0

125. Dienal conformer 8 (2*Z*,4*E*-*cis*,*cis*) (-500.393351)

6	-0.392525	-0.136557	0.000215
6	-1.140057	-1.274474	0.000310
1	-0.919589	0.813116	0.000281
1	-0.626042	-2.234406	0.000324
6	-2.579991	-1.403944	0.000542
6	-3.631756	-0.524472	0.000247
1	-2.896711	-2.447916	0.000992
1	-4.623272	-0.975702	0.000480
6	-3.674486	0.934159	-0.000531
8	-2.730170	1.720457	-0.000572
1	-4.707002	1.342217	-0.001141
6	1.067239	-0.058582	0.000070
6	1.660671	1.221125	0.000544
6	3.046794	1.374852	0.000487
6	3.874237	0.248911	-0.000082
6	3.303223	-1.030535	-0.000604
6	1.919767	-1.183668	-0.000530
1	1.018050	2.098280	0.000973
1	3.480037	2.371672	0.000876
1	4.955106	0.363500	-0.000140
1	3.942200	-1.910015	-0.001083
1	1.499882	-2.185286	-0.000985

$E_{(MeCN)}$ = -500.506065
NImag = 0

126. Enone 3*E*-*cis* Conformer (-270.570090)

6	-1.087442	0.147761	-0.000014
8	-1.265865	1.359755	-0.000019
6	0.273694	-0.458937	0.000003
6	1.387354	0.291924	-0.000002
1	0.338008	-1.547078	0.000019
1	1.258171	1.374901	-0.000017
6	2.789654	-0.229565	0.000014
1	3.338005	0.135853	0.879330
1	2.824346	-1.324170	0.000036
1	3.338011	0.135817	-0.879313
6	-2.255239	-0.822776	0.000004
1	-2.209485	-1.475141	0.882314
1	-3.198918	-0.273269	-0.000142
1	-2.209340	-1.475393	-0.882110

$E_{(MeCN)}$ = -270.631961
NImag = 0

Optimized coordinates for the addition TSs (pathway-5) computed at the B3LYP/6-31+G level of theory**

127. **5a**-A-*c*‡ (-1018.891451)

6	2.025147	-0.112608	1.138103
6	1.637409	-0.174454	-0.219782
6	2.645118	-0.472180	-1.165189
6	3.969605	-0.677982	-0.779749
6	4.336516	-0.582656	0.566718
6	3.354418	-0.302077	1.520979
6	0.229370	-0.048857	-0.649092
16	-0.595907	1.512745	-0.495420
6	-0.606435	1.998465	1.258687
6	0.527223	2.831050	-1.131950
6	-1.146525	-1.569345	0.122307
6	-2.444902	-1.388688	-0.368011
6	-3.367565	-0.494230	0.252622
8	-3.059434	0.271842	1.201203
6	-0.347264	-2.777270	-0.306112
6	-4.804933	-0.461081	-0.253891
1	1.505470	2.753594	-0.653401
1	0.621167	2.682801	-2.208837
1	0.409439	2.059606	1.650767
1	-1.234635	1.260855	1.762003
1	0.062823	-0.323677	-1.691882
1	-0.731346	-3.661194	0.219540
1	-0.452350	-2.966408	-1.380240
1	0.715530	-2.687519	-0.069349
1	-2.758857	-1.933753	-1.255436
1	-4.978430	-1.138396	-1.095321
1	-5.478260	-0.733128	0.566584
1	-5.062713	0.560771	-0.554429
1	-1.097979	2.973030	1.300716
1	0.069862	3.803103	-0.930128
1	2.376700	-0.541964	-2.216585

1	4.718556	-0.905903	-1.533421
1	5.368039	-0.737380	0.868465
1	-0.978637	-1.240689	1.145271
1	1.273436	0.040095	1.905217
1	3.619072	-0.251045	2.573711

$E_{(MeCN)}$ = -1019.029296
NImag = 1 (-245.0)

128. **5a**-A-$t^{‡}$ (-1018.880675)

6	-2.073815	-2.191794	-1.598641
1	-2.844427	-1.581971	-1.125677
1	-1.830265	-1.794137	-2.584582
16	-0.517133	-2.150932	-0.612096
6	-1.139814	-2.911603	0.929720
1	-1.996926	-2.373138	1.333951
1	-0.317319	-2.913252	1.644596
6	0.015790	-0.476851	-0.268145
1	0.779897	-0.349304	-1.035129
6	1.368647	-0.365207	1.214155
6	0.592965	-0.135210	2.494689
1	1.265456	-0.264878	3.351459
1	0.192791	0.882339	2.537713
1	-0.245215	-0.826630	2.624687
6	2.304198	0.619487	0.815298
1	2.254892	1.615245	1.248138
6	3.205532	0.349796	-0.252380
6	4.272957	1.383537	-0.597715
1	4.202735	2.289065	0.013235
1	5.262824	0.936021	-0.452440
1	4.196217	1.653842	-1.656920
8	3.147813	-0.703634	-0.939322
1	-1.414038	-3.940845	0.687933
1	-2.391768	-3.233794	-1.685535
6	-0.978473	0.614650	-0.213923
6	-0.657218	1.831625	-0.853689
6	-1.499297	2.941147	-0.764356
6	-2.698621	2.866069	-0.051336
6	-3.034527	1.669525	0.590150
6	-2.182082	0.567292	0.521130
1	0.264514	1.897972	-1.423028
1	-1.219755	3.864631	-1.263855
1	-3.359031	3.725832	0.009217
1	1.723888	-1.385384	1.066088
1	-2.453609	-0.330280	1.067941
1	-3.956695	1.597887	1.160567

$E_{(MeCN)}$ = -1019.024862
NImag = 1 (-351.5)

129. **5b**-A-$c^{‡}$ (-1018.881931)

6	0.612548	2.632937	-1.476168
1	1.627473	2.523692	-1.090781
1	0.553939	2.241620	-2.492837
16	-0.566616	1.658765	-0.470552
6	-0.426746	2.541327	1.124149
1	0.606892	2.626908	1.456881
1	-1.020776	1.980366	1.843991
6	0.043048	0.004886	-0.304834
1	-0.483999	-0.513644	-1.110365
6	-1.137405	-0.981780	1.061102
6	-0.502787	-0.817665	2.424139
1	-0.870643	0.069586	2.951785
1	-0.765077	-1.685557	3.042448
1	0.589012	-0.772260	2.373756
1	-0.824551	-1.890474	0.548112
6	-2.497460	-0.643500	0.869678
1	-3.018771	-0.046184	1.615295
6	-3.157084	-1.000688	-0.341257
6	-4.649376	-0.713954	-0.480590
1	-5.075052	-0.221906	0.399936
1	-4.823607	-0.088872	-1.363781
1	-5.179029	-1.658539	-0.647321
8	-2.559020	-1.532072	-1.312050
1	-0.865594	3.530631	0.977092
1	0.294414	3.678222	-1.461011
6	1.480334	-0.294018	-0.236531
6	1.944610	-1.431674	-0.939381
6	3.272634	-1.845769	-0.856702
6	4.194558	-1.130958	-0.084246
6	3.758084	-0.004438	0.618334
6	2.423673	0.400448	0.554727
1	1.244400	-1.988343	-1.556517
1	3.591634	-2.725644	-1.408781
1	5.231246	-1.448240	-0.027267
1	4.456457	0.557394	1.232989
1	2.117853	1.256665	1.147085

$E_{(MeCN)}$ = -1019.024746
NImag = 1 (-337.0)

130. **5b**-A-$t^{‡}$ (-1018.891022)

6	-2.208116	2.587840	-0.849633
1	-2.514104	1.672238	-1.359252
1	-2.897908	2.820310	-0.037268
16	-0.538765	2.342644	-0.108389
6	0.411935	2.084717	-1.645490

1	-0.167813	1.472391	-2.338116
1	1.358426	1.580394	-1.392768
6	-0.522440	0.844850	0.848439
1	-0.922538	1.168937	1.810073
6	1.491122	0.451276	1.424728
6	1.283008	0.497752	2.926225
1	0.682654	-0.350567	3.273801
1	2.257005	0.435128	3.427197
1	0.801207	1.423329	3.257651
1	1.901746	1.366168	1.000427
6	1.987544	-0.729120	0.845379
1	1.852589	-1.671341	1.370587
6	2.656464	-0.741547	-0.409889
6	3.301855	-2.042408	-0.873827
1	3.127519	-2.875527	-0.186741
1	2.919580	-2.307161	-1.866131
1	4.381575	-1.887022	-0.978700
8	2.761145	0.263156	-1.165767
1	0.588754	3.076307	-2.068860
1	-2.154658	3.426380	-1.548569
6	-1.192301	-0.361540	0.326731
6	-2.232517	-0.959009	1.070316
6	-2.837885	-2.142668	0.649932
6	-2.424910	-2.760949	-0.535625
6	-1.386173	-2.193276	-1.276467
6	-0.762776	-1.018639	-0.845675
1	-2.569078	-0.481577	1.987813
1	-3.638547	-2.577379	1.242095
1	-2.899845	-3.678738	-0.869757
1	-1.039927	-2.677131	-2.185637
1	0.075579	-0.626375	-1.408349

$E_{(MeCN)}$ = -1019.024746
NImag = 1 (-265.7)

Optimized coordinates for the torsional TSs computed with the *E-trans,trans* dienal conformer along pathway-2 obtained at the B3LYP/6-31+G* level of theory

131. **2a**-R‡ (*E-trans*,*trans* dienal) Conformer 1 (-1248.67936284)

6	0.429353	2.034640	-0.416179
6	1.384896	1.380915	0.382266
6	1.957280	2.079045	1.458137
6	1.578519	3.395130	1.738466
6	0.635148	4.037332	0.933532
6	0.064304	3.354084	-0.145996
6	1.794324	-0.051250	0.145041
16	2.575582	-0.154407	-1.591044
8	1.942578	-4.297911	2.017569
6	-0.697504	-0.733390	0.423969
6	-1.681594	-0.970023	-0.465339
6	-3.099774	-0.604106	-0.345075
6	-3.948240	-0.780260	-1.455995
6	-5.299759	-0.435563	-1.402165
6	-5.842562	0.093699	-0.228430
6	-5.016801	0.266592	0.889095
6	-3.667748	-0.078162	0.833791
6	3.533298	-1.708237	-1.473030
1	4.210601	-1.669091	-0.617053
1	2.829698	-2.532279	-1.339458
1	4.548544	0.923409	-0.675287
1	3.491805	2.056524	-1.576064
1	2.632860	-0.316831	0.795357
1	1.025217	-1.747828	2.435483
1	4.537873	0.914446	-2.473129
1	4.084132	-1.825435	-2.409584
1	1.507816	-3.743355	0.105961
1	-0.913084	-0.206169	1.352350
1	-1.424958	-1.500558	-1.384955
1	0.753282	-1.838872	-0.638504
1	-3.052520	0.046113	1.720474
1	-5.430135	0.664181	1.813118
1	-6.895339	0.359717	-0.179673
1	-5.929350	-0.584966	-2.276203
1	-3.536791	-1.196499	-2.373797
1	2.689046	1.582473	2.091311
1	2.021874	3.914900	2.583651
1	0.341011	5.061422	1.147416
1	-0.677902	3.843873	-0.770624
1	-0.045982	1.505398	-1.236636

$E_{(MeCN)}$ = -1248.919727
NImag = 1 (-30.0)

132. **2a**-R‡ (*E-trans*,*trans* dienal) Conformer 2 (-1248.67079577)

6	-2.966136	0.130017	1.179555
6	-2.697989	-0.236596	-0.151045
6	-3.774522	-0.426686	-1.028549
6	-5.092913	-0.252970	-0.594377
6	-5.347480	0.096987	0.732298
6	-4.280697	0.283931	1.618887
6	-1.293684	-0.417914	-0.656447
16	-0.536227	-1.922512	0.287372
6	3.937441	1.060544	-1.570908
6	0.713931	-1.241311	0.286631
6	1.100975	-2.132103	1.418627
6	1.538241	-3.443704	1.197229

6	-1.862913	-3.178266	0.268839
6	-0.287798	0.871031	-0.594869
6	-0.826384	2.083052	0.062045
6	-1.274756	3.189224	-0.679144
8	-1.734428	4.270764	-0.251395
6	1.068425	0.559853	-0.012652
6	2.217124	0.470307	-0.722440
6	3.579889	0.318797	-0.198615
6	4.628050	0.015396	-1.091900
6	5.937810	-0.161282	-0.644192
6	6.238470	-0.034622	0.714918
6	5.213316	0.280471	1.615332
6	3.905568	0.457184	1.167714
6	0.601833	-2.679334	-0.921374
1	0.074746	-2.873002	-1.859488
1	1.422905	-1.976395	-1.069015
1	-2.247437	-3.315466	-0.744368
1	-2.659969	-2.829336	0.925850
1	-1.328237	-0.799006	-1.685093
1	-0.824890	2.149785	1.148912
1	-1.440536	-4.110741	0.654561
1	0.976514	-3.611087	-0.489934
1	-1.198659	3.051246	-1.792532
1	1.105970	0.515862	1.076903
1	2.149822	0.534981	-1.811072
1	-0.162177	1.095066	-1.664196
1	3.133267	0.730886	1.881156
1	5.438197	0.402557	2.672302
1	7.258132	-0.165356	1.067687
1	6.724985	-0.391380	-1.358300
1	4.406989	-0.076050	-2.153956
1	-3.581666	-0.684548	-2.067992
1	-5.913922	-0.387625	-1.293479
1	-6.369729	0.236637	1.073662
1	-4.472129	0.576542	2.647589
1	-2.148391	0.309026	1.870097

$E_{(MeCN)}$ = -1248.914613
NImag = 1 (-35.0)

133. **2b**-R‡ (*E-trans*,*trans* dienal) (-1248.67516533)

6	4.739287	0.337577	-0.702402
6	3.664591	-0.163970	0.059071
6	3.951872	-0.647106	1.352818
6	5.248998	-0.612918	1.860824
6	6.302147	-0.100427	1.093321
6	6.039057	0.371733	-0.195203
6	2.315511	-0.158263	-0.521803
6	1.152599	-0.466036	0.088820
6	-0.193362	-0.547642	-0.590040
6	-0.717262	-1.934737	-0.584700
6	-0.969462	-2.614958	-1.785420
8	-1.411793	-3.773152	-1.952979
6	-1.167767	0.559287	0.102977
16	-1.481720	1.917997	-1.164416
6	-2.399153	3.222972	-0.275562
6	-2.511625	0.112108	0.607635
6	-3.413195	-0.590262	-0.212095
6	-4.639022	-1.019444	0.303368
6	-4.972372	-0.769085	1.637618
6	-4.078201	-0.079873	2.461998
6	-2.857206	0.361604	1.945062
6	0.144867	2.729653	-1.331269
1	0.519566	3.034721	-0.351486
1	0.830976	2.011332	-1.779744
1	-2.521550	4.073887	-0.951989
1	-1.859644	3.519283	0.627560
1	-0.627282	1.078705	0.903937
1	-0.882880	-2.438397	0.365781
1	-3.374725	2.810035	-0.014678
1	0.019779	3.592171	-1.990598
1	-0.743832	-2.001107	-2.704409
1	-0.065494	-0.263234	-1.648376
1	1.150059	-0.755983	1.140768
1	2.283311	0.098674	-1.583573
1	4.547971	0.700301	-1.710932
1	6.847081	0.761981	-0.809528
1	7.313152	-0.080215	1.491764
1	5.442794	-0.998239	2.859164
1	3.156960	-1.070265	1.960638
1	-2.156766	0.884551	2.593976
1	-4.325718	0.110189	3.503015
1	-5.921779	-1.117609	2.035914
1	-5.321953	-1.571986	-0.335694
1	-3.149981	-0.822826	-1.237146

$E_{(MeCN)}$ = -1248.918757
NImag = 1 (-17.6)

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Full list of citations for *Gaussian03* (Reference 41 in the text)

Gaussian03:

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